


November 2001

# Science & Technology

REVIEW



U.S. Department of Energy's  
Lawrence Livermore  
National Laboratory

A large, artistic illustration of a welding process. A bright, glowing blue cube is positioned in the upper center, with a beam of light or energy directed downwards from it. At the point of contact, a massive burst of bright orange and yellow sparks erupts, radiating outwards in all directions. The background is dark, with some faint, glowing green spots. The overall effect is one of intense energy and scientific precision.

## Welding Science at the Atomic Level in Real Time

*Also in this issue:*

- Monitoring Enhanced Oil Recovery
- Probing Liquid Water's Surface with X Rays
- Designing New Targets for Fusion Power

## About the Cover

Welding—the process of melting and fusing together two pieces of material—has been around a long time and is fundamental to industrial civilization. Yet, until recently, little was known about the basic science of welding—and thus, about how to strengthen welds and make them last longer. Basic welding science research at Livermore is, however, changing all that. With the help of synchrotron radiation, materials science researchers are now able to “see” and analyze the welding process at the atomic level as it occurs. The effects of this award-winning research are already being seen in process improvements that make welds stronger and safer. Turn to p. 4 for the full report.



Cover design: Lew Reed

## About the Review

Lawrence Livermore National Laboratory is operated by the University of California for the Department of Energy's National Nuclear Security Administration. At Livermore, we focus science and technology on assuring our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published 10 times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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### Digital mammography gets FDA approval

Fischer Imaging Corporation of Denver, Colorado, has received Food and Drug Administration approval for its digital mammography system, which was initially developed in collaboration with Lawrence Livermore scientists and engineers under a Cooperative Research and Development Agreement between 1993 and 1996.

FDA approval of SensoScan, the Fischer Imaging system, means that the federal agency has found the digital system to be safe and effective for use in the same clinical applications as traditional mammography. FDA approval also means that SensoScan becomes available for regular clinical use to treat patients. Previously, it could only be used in a research setting.

Traditional mammography technology uses film to record the x-ray image of breast tissue. SensoScan records the image electronically. Thus, tissue images can be acquired at one location and rapidly transmitted to another site for interpretation.

Better yet, with digital mammography, computers can now be used to help diagnose and evaluate the high-fidelity digital tissue images. According to Livermore mechanical engineer Clint Logan, who heads the collaboration with Fischer, image variables such as contrast and brightness can be adjusted on computer display, not fixed by film chemistry and exposure. Thus, the possibility of human error or misinterpretation decreases.

The Laboratory's ability to assist in the development of digital mammography grew out of work performed for ballistic missile defense, specifically the X-Ray Laser Program. When the U.S. ended that program, the Livermore team applied the materials analysis and characterization tools and expertise developed for the x-ray laser to other technologies, including digital mammography.

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### Livermore cosponsors tribes' energy conference

In late August, the Laboratory cosponsored a two-day conference on energy solutions with the Council of Energy Resource Tribes (CERT). The conference attracted 350 participants representing nearly 50 American and Canadian Indian tribes, private industry, the University of California, and the Department of Energy.

This is the 20th year that CERT has held the conference and the first time it has asked a national laboratory to be a cosponsor, according to Livermore's Karen Kiernan, who coordinated Livermore's involvement in the conference.

CERT is a coalition of 44 American Indian tribes and 4 Canadian affiliate members that own a substantial share of North America's energy reserves.

The conference, held in San Jose, California, included workshops on Indian energy solutions such as conservation, natural resource strategies, and tribal policies.

The tribes are working to have a much stronger technical and managerial role in developing energy resources on tribal lands than in the past, when they principally received only royalties.

The conference also included the American Spirit Awards dinner, a fund-raiser for CERT's scholarship fund. At this dinner, Steve Grey, representative for the DOE-Livermore American Indian Program field office, presented two scholarships to essay winners on behalf of the Laboratory.

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### Laboratory-Russia to partner on dialysis equipment

Following lengthy negotiations led by Laboratory representatives, the first joint commercial venture between a former Russian weapons manufacturer and a U.S. firm has been formally signed.

Avangard Electromechanical Plant in Russia and Fresenius Medical Care in the U.S. will establish a commercial medical equipment manufacturing facility in Sarov, Russia. The new company, called FRESAR, will produce high-quality, low-cost kidney dialysis equipment.

The project is part of the National Nuclear Security Administration's (NNSA's) Nuclear Cities Initiative (NCI), which seeks to reduce the risk of nuclear proliferation by helping create civilian jobs for displaced weapons workers in the former Soviet Union. The project also receives funding from NNSA's Initiatives for Proliferation Prevention program.

FRESAR will build assembly lines for disposable medical products used in Fresenius kidney dialysis equipment. The lines are expected to be fully operational by the end of 2003, with products to be marketed by Fresenius in Russia and other European countries.

The venture was spearheaded by Ann Heywood, leader of the Laboratory's Russian medical technologies work in support of NCI, and Jim Trebes of the Physics and Advanced Technology Directorate's Medical Technology program. The project is managed by the Nonproliferation, Arms Control, and International Security Directorate.

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# Fundamental Science Supports National Needs

**E**XPLORATORY, basic scientific research is key to the Laboratory's success in fulfilling its missions. Our primary mission is to provide for national security in a changing world. At the same time, we must also respond to an array of enduring national needs. We are improving energy security and environmental management, advancing bioscience to improve human health, and pursuing breakthroughs in science and technology. In all of this work, we are pushing the frontiers of science and often must know the basics before we can proceed with the more complex.

Stockpile stewardship provides a particularly dramatic example of the need for basic science. Few other institutions are responsible for maintaining an aging nuclear stockpile, one for which no new weapons are being manufactured. When the weapons program started, no one knew what would happen to plutonium and other materials in the weapons as they age. Today, fundamental science plays a critical role in evaluating the effects of aging on plutonium.

The Department of Energy and its National Nuclear Security Administration (NNSA) recognize the importance of fundamental research. In addition to the considerable funding that comes to the Laboratory through NNSA's Stockpile Stewardship Program each year, DOE's Office of Basic Energy Science (BES) funds an array of projects, including two of the four research endeavors addressed in this issue. The research described in the lead article on the science of welding, which begins on [p. 4](#), was funded in part by BES, as was the work on hydrogen bonding in liquid water, described in the research highlight beginning on [p. 20](#). The results of both projects have ramifications that extend far beyond the laboratories where the experiments took place.

Welding is critical to all aspects of national security. Virtually all systems used in the defense of our country are welded. And the fabric of the world's civilian infrastructure, including highways and bridges, power generation and distribution, and high-rise construction, depends on effective, robust welds. Reliable welds also help protect the environment. The Alaska Pipeline, for example, delivers millions of barrels of oil a year across the fragile Alaskan tundra through welded pipes.

Welding dates back centuries to when humans first began to work with metal. Yet, only in recent years have scientists had the tools that allow them to take a close look at this

technology in real time. Synchrotron radiation, a tool used to unlock the structure of proteins, is being applied to the science of welding with the goal of making welds safer and more reliable. Livermore experimental results indicate potential problems with existing welding technology. To counteract potential safety problems related to weld integrity, developers are incorporating Livermore data into the design of new welding electrodes to create more reliable welds.

Until recently, hydrogen bonding in liquid water has been difficult to examine experimentally. Livermore's work on this basic problem also takes advantage of synchrotron radiation, using it to determine for the first time the distance between hydrogen atoms and oxygen atoms at the surface of liquid water. Details of hydrogen bonding in liquids are important for almost all biological or environmental research. DNA is a double helix because of hydrogen bonding. The structure of proteins, which exist in the liquid water of our cells, is defined in part by hydrogen bonding. Any system that involves liquid water is affected by the way that hydrogen bonds. The research presented here is helping to unravel the secrets of hydrogen-bonded materials.

As long as Lawrence Livermore is performing science in the national interest, basic research will continue.

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■ Hal Graboske is associate director of Chemistry and Materials Science.



# Welding Science

## A New Look at a Fundamental Technology

*Livermore experiments allow a second-by-second examination of what occurs during welding.*

**W**ELDS—the melting and fusing together of two pieces of material to make one—hold together much of the industrial world. Your safety while driving in a car depends in part on the reliability of more than 3,000 welds. If a weld were to fail, the results could be catastrophic. Welds make possible airplanes, metal bridges, office buildings, and high-pressure tanks as well as all sorts of high-technology devices. Welding is the most widely used method for joining metals and is typically stronger, lighter, and cheaper than other joining methods such as riveting and bolting.

Forge welding has been around almost since people began to work with metals. Then, in the late 19th century, Sir Humphrey Davy discovered the electric arc, and modern welding was born. The materials that welders use have changed over the years and today include not just metals but also polymers, ceramics, and composite and engineered materials. Lasers, electron beams, and plasma arcs supplement traditional electric and torch welding methods. Yet for all this history, basic knowledge about the welding process is surprisingly sparse. Conventional inspection techniques are not adequate

to indicate how a weld evolves in time. Welding may be old, but the science of welding is in its infancy.

Livermore has a vital interest in knowing all it can about welding. Dependable welds are important for maintaining the performance and safety of nuclear weapons. Welds will also play a key role in the success of the Department of Energy's planned repository for long-term storage of nuclear wastes, which will potentially be located at Yucca Mountain in the Nevada desert. Waste canisters will have three layers of containment: a convenience can inside an inner can inside an outer can. The lids of the inner and outer cans will be welded shut. The canistered waste must remain impervious to attack by air, moisture, and the surrounding environment for thousands of years. All told, more than 100 miles of welds will be required at the repository.

Metallurgist John Elmer, Livermore's expert on welding, has been researching details of the welding process since the early 1990s with physical chemist Joe Wong, whose

specialty is synchrotron x-radiation experiments. They are currently working with another metallurgist, Todd Palmer. The three are also collaborating with colleagues at Pennsylvania State University and Oak Ridge National Laboratory.

Over the last several years, the team has succeeded in producing maps of the microstructural changes that occur in and around the weld area as a metal melts and resolidifies. More recently, their experiments have revealed second-by-second changes in a metal's microstructure during welding. In contrast, conventional diagnostic techniques can examine the material only before and after welding or can derive information about changes only indirectly and after the fact. "These experiments at Livermore have given us the first real-time look at the welding process," says Lou Terminello, division leader in the Chemistry and Materials Science Directorate.

### Welds Take the Heat

When two pieces of material are being welded together, high heat

rapidly melts the solid material, which quickly cools and solidifies again as the heat source moves away. Adjacent to the immediate weld area, or fusion zone, is the heat-affected zone (HAZ). As the name HAZ implies, the material there is affected by the high heat of the welding process but does not melt.

Heat causes changes in the material. The three well-known basic phases of a material are gas, liquid, and solid. But for many materials, multiple solid phases exist at various temperatures or at various combinations of temperature and pressure. At sea level—1 atmosphere—plain old H<sub>2</sub>O may form several kinds of ice, each of which is a different solid phase. Iron undergoes three solid-state phase transformations as its temperature increases from room temperature to 1,535°C, where it melts. Carbon also has several solid phases, including graphite and diamond. No one would confuse graphite and diamond. Each one is still carbon, but their crystal structures are very different.

When a material is welded, its crystalline structure changes. It is these microstructural changes that interest

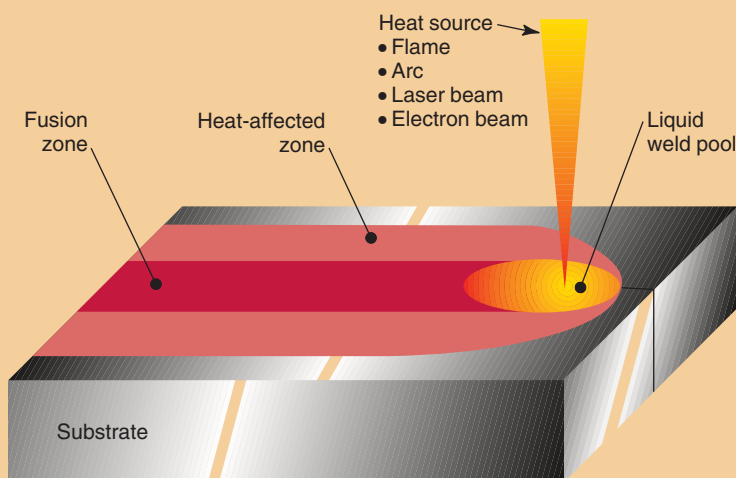


Illustration of a fusion weld. A liquid weld pool is created through the interaction of an intense heat source and the substrates being joined. Melting on the front side of the weld pool eliminates the interface between the materials, while solidification on the back side of the weld pool fuses the substrates together to create a solid joined part. Surrounding the fusion zone is a heat-affected zone, where the substrate is heated to temperatures up to the melting point of the metal being joined. Solidification in the fusion zone and solid-state phase transformations in the heat-affected zone are responsible for dramatic changes in the microstructure and properties of the welded joint.



Elmer. They can affect the strength of the material as well as its corrosion resistance, ductility, and mechanical properties. Any or all of the changes could either enhance the quality of the weld or reduce the weld's integrity. "We want to be able to understand the welding process by modeling it and then predict the changes that will occur," says Elmer. "But first, we need to gather real experimental data during welding to understand the fundamental properties of the process."

### Synchrotron Is Key

Joe Wong has been performing experiments with synchrotron radiation to examine materials for the past two decades. He and others helped to develop the experimental facility at the Stanford Synchrotron Radiation Laboratory back in 1977.

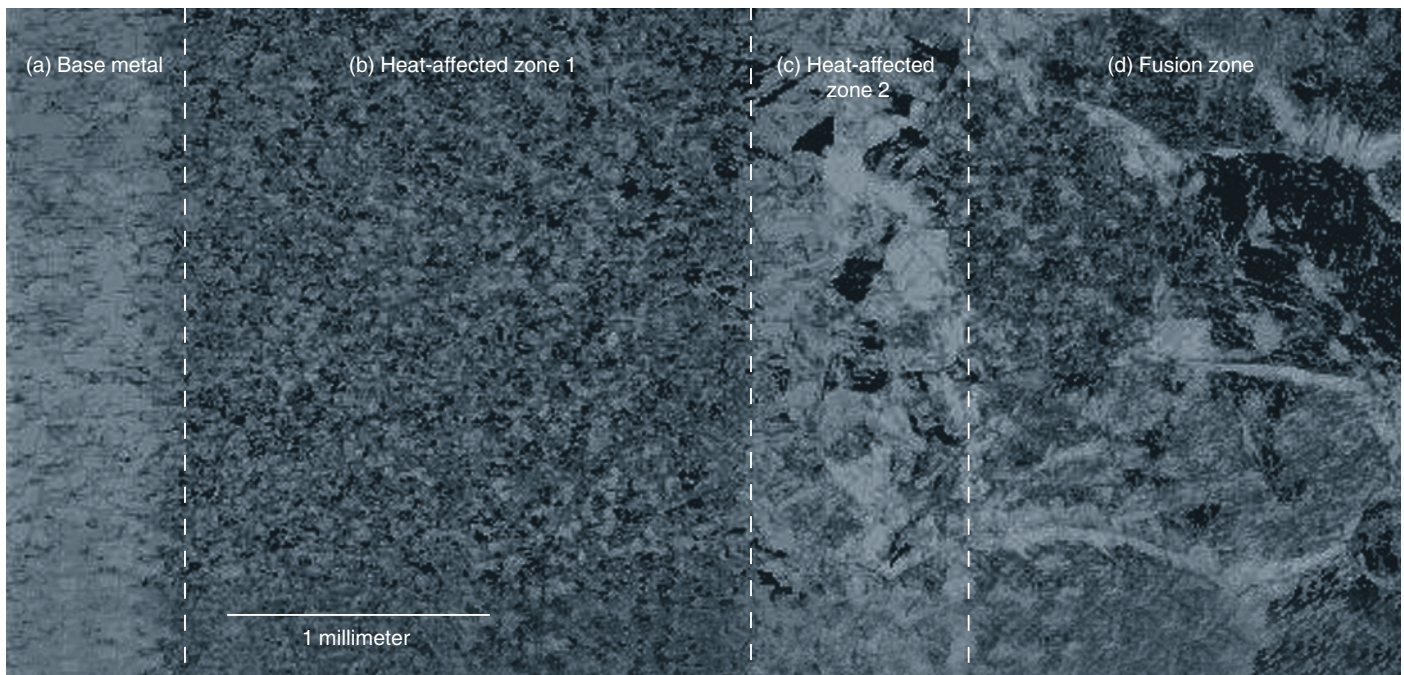
Synchrotron radiation is a particularly intense form of electromagnetic radiation. Highly energetic charged particles traveling at almost the speed of light and deflected in a magnetic field emit synchrotron radiation. This intense, highly collimated radiation—millions of times more powerful than that from a conventional x-ray tube—can probe the atomic structure and electronic states of matter. Experiments that would have taken hours with an x-ray tube source take milliseconds instead.

Synchrotron radiation spans the electromagnetic spectrum from infrared to hard x rays. X rays are ideal for probing matter because the wavelength of x-radiation is about the same size as an atom. Thus, with synchrotron x rays, the team can make direct observations of phase transformations in welds,

watching microstructural changes as they evolve.

Synchrotron radiation sources at Stanford and elsewhere around the world are used by scientists working in many fields—by materials scientists like Elmer and Wong to study the dynamic properties of solid and amorphous materials, by biomedical researchers to study proteins and other large biomolecules, by medical workers for coronary angiography and other forms of imaging, and by geologists for structure characterizations and trace-element analyses of minerals.

The Livermore team is using x rays from the 31-pole x-ray "wiggler" at Stanford Synchrotron Radiation Laboratory for their experiments. In this device, an x-ray beam wiggles between an array of 31 magnetic poles, gathering intensity along the way. By carefully



Room-temperature top view of the microstructure of titanium from the fusion zone, through the heat-affected zone, and into the base metal (30 times magnification): (a) the base metal, (b) the small-grained portion of the heat-affected zone where the gamma phase has partially transformed to the beta phase, (c) the large-grained portion of the heat-affected zone where gamma-phase titanium has fully transformed into the beta phase, and (d) the fusion zone. Note the dramatic changes in grain structure.



directing this small, intense synchrotron beam at a given location in a weld, they can obtain an x-ray diffraction pattern to identify the phases present in the material at that location during the welding process. The x-ray diffraction pattern depends on the atomic structure of the material. “The diffraction pattern is the fingerprint of a material’s crystal structure,” says Wong. “Liquid is chaotic with no long-range order,” he continues, “so there is no diffraction.”

### From Simple to Complex

The team’s first experiments examined titanium welds. Titanium is popular in manufacturing because of its corrosion resistance and light weight. Also, titanium has two well-characterized solid-phase transitions at ambient air pressure before it melts. In pure titanium, the alpha phase exists

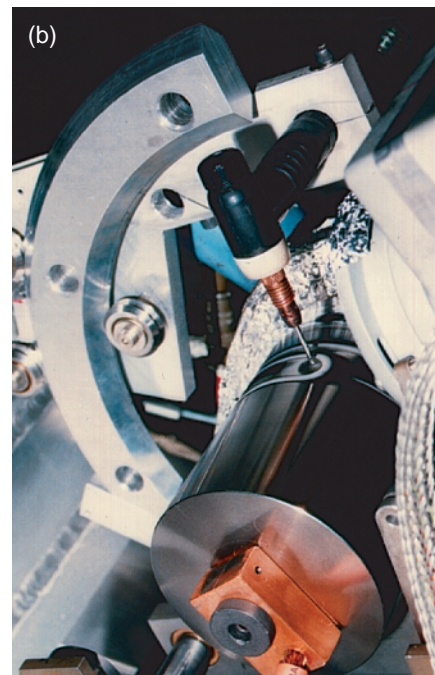
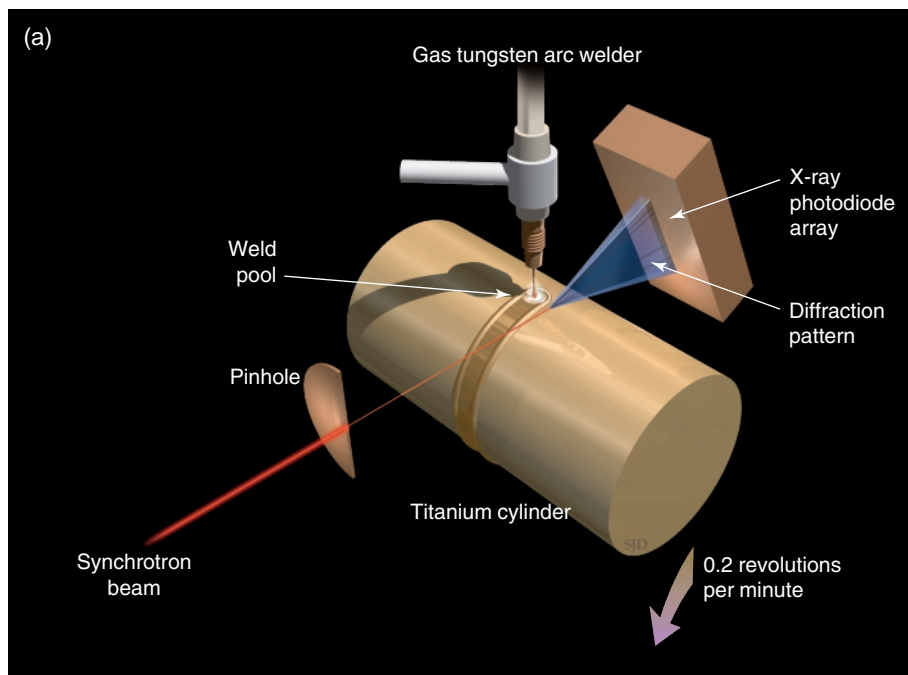
from room temperature to 882°C. At these temperatures, titanium has a hexagonal-close-packed crystalline structure. At 882°C, pure titanium’s crystalline structure changes to the beta (body-centered-cubic) phase, which it maintains until it reaches the liquid phase at 1,670°C. As the liquid titanium cools, the phase transformations are reversed. Because these phase transformations occur over such a wide temperature range, titanium is a relatively easy material to study.

Using the experimental setup shown in the figure below, a metal bar rotates under a gas tungsten arc, taking 6 minutes for a full revolution. An intense x-ray beam from the synchrotron source passes through a pinhole to allow researchers to resolve features as small as 180 micrometers. During welding, the x-ray beam is

aimed at specific points around the heat source. A silicon photodiode linear array detector records the diffraction patterns during the experiment.

The team maps phase transformations by performing a series of sequential linear scans from the centerline of the weld and out into the HAZ. In every row, 30 to 40 x-ray diffraction patterns are collected, spaced 0.25 millimeters apart. Each row requires one revolution of the cylinder. After completion of the first row, the welding heat source is moved 1 millimeter from its previous position to collect data in the next row, and so on.

This spatially resolved x-ray diffraction (SRXRD) technique is unique to Livermore for the study of welding. “Spatial resolution is the key to collecting useful in situ phase transformation data during welding,” says Elmer.



(a) A rendering of (b) the experimental setup for real-time investigations of welds using synchrotron radiation. The x-ray beam enters from the lower left through a pinhole to provide spatial resolution of 180 micrometers. During welding, this spatially resolved beam is aimed at a specific location of the weld where diffraction takes place. The diffracted beams are captured in real time using a silicon photodiode linear array detector. The weld is produced by a gas tungsten arc on a revolving solid bar of the material being studied.

The grain structure of commercially pure titanium—or any solid material for that matter—changes during welding. It is subjected to peak temperatures hundreds of degrees higher than the melting point, followed by rapid cooling. These temperature fluctuations alter the microstructure of the material nonuniformly to create the HAZ adjacent to the weld fusion zone. Solid-state phase transformations that occur in the HAZ create gradients of both microstructure and properties between the liquid metal in the fusion zone and the unaffected base metal farthest from the weld. Within the HAZ, the most severe microstructural changes occur close to the fusion zone, where the peak temperatures are the highest.

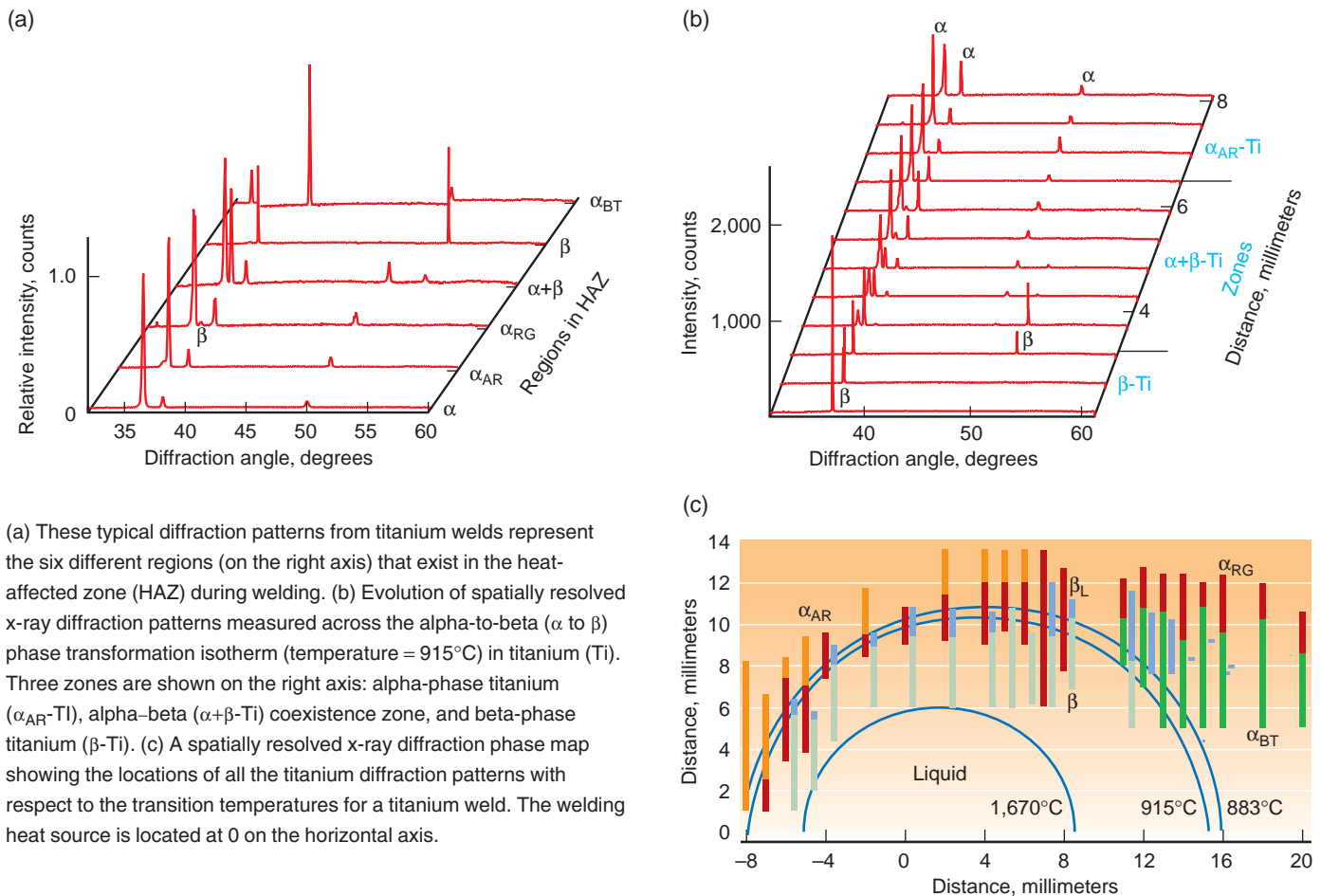
Researchers had suspected for some time that annealing and recrystallization occur in the colder portions of the HAZ in titanium. They also knew that both partial and complete alpha-to-beta transformations take place in the hotter portions of the HAZ. But what they had not been able to determine was the exact size and location of these regions.

Using SRXRD, the Livermore team found six regions in the HAZ around the liquid titanium weld pool, each with an identifiable diffraction pattern. From their diffraction data, they could follow the evolution of the phase transformations, at various locations and at various temperatures. This research resulted in a diffraction map of the HAZ [part (c) of the figure

below] that shows the location of all the phases with respect to the transition temperatures.

“Titanium was a good place to start with our experiments,” says Elmer. “But steels are welded much more frequently.” So their next sets of experiments dealt with carbon–manganese steel and stainless steels. While these alloys have more complex phase changes than pure metals, their phase transformations can be studied with the SRXRD technique.

Duplex stainless-steel alloys consist of austenite and ferrite solid phases, each of which has different crystal structures and magnetic properties. Here, they found five principal phase regions between the



liquid weld pool and the unaffected base metal that contribute to the final microstructure observed in the HAZ.

### Changes over Time

Phase mapping experiments performed using the SRXRD method are useful for observing phase changes under quasi-steady-state heating and cooling conditions. The next step was to examine the changes that occur at a single spot as a function of time. Wong developed a time-resolved x-ray diffraction (TRXRD) technique that takes a set of x-ray diffraction patterns at a single location adjacent to or within a stationary spot weld. When the detector is clocked for durations of tens to hundreds of milliseconds, phase transformation may be observed on a much shorter time scale than is possible with moving welds. Changes in the diffraction pattern show directly how phase changes are taking place as a function of time and temperature. As the temperature goes up and then down, the metal at the weld becomes liquid and then solidifies. With TRXRD, the Livermore team has been

able to examine the solidification and subsequent solid-state phase transformations in a number of different materials for the first time.

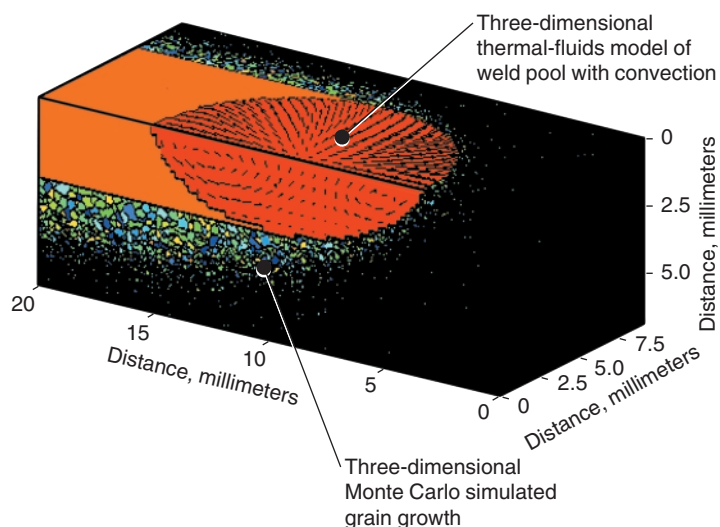
For example, TRXRD has proved useful for examining the solidification behavior of austenitic stainless steels. In these stainless steels, the presence of residual ferrite in the austenitic microstructure affects the integrity of welds. Researchers have long been interested in understanding how residual ferrite in the microstructure evolves. For more than 50 years, those who work with welds have known that the composition of the weld is important and have developed methods for assuring that the austenite-ferrite ratio was appropriate for each specific need. Numerous studies have examined the rate of solidification, which affects the microstructure and relative percentage of austenite and ferrite in the final weld.

But Livermore was the first to make direct observations of the ferrite and austenite phases and the dynamics of this transformation. The Livermore team found directly, for the first time,

that ferrite is the first phase to solidify from the liquid weld pool in a 304 stainless-steel alloy. The ferrite phase existed as the only solid phase for 500 milliseconds before beginning to transform into the austenite phase. The ferrite-to-austenite transformation took an additional 200 milliseconds of cooling, during which both phases coexist. The combined results showed that the majority of the ferrite phase transformed to the austenite phase by the time the weld had cooled to a temperature of 1,100°C.

### Beginning to Predict

Elmer and Palmer have also worked with modeling experts at Pennsylvania State University, where a research group has spent many years developing models to predict the temperatures present throughout a weld. By combining the results of the SRXRD experiments with the modeling results, the evolution of observed phase transformations can be more fully understood. As part of their collaboration, they performed three-dimensional Monte Carlo simulations



Three-dimensional Monte Carlo simulation of grain-size evolution in welds.



Infrared image of a duplex stainless-steel weld obtained in real time during a synchrotron experiment.

of the growth of grains during gas tungsten arc welding of titanium, shown in the [figure on the left on p. 9](#).

The Livermore–Penn State collaboration has continued to study phase transformations in duplex stainless steels. SRXRD observations of the phases present around the weld pool of an arc-welded 2205 duplex stainless steel have been combined with the results of a Penn State heat-transfer model to produce a thorough map of the

phase transformations occurring in the heat-affected zone. An infrared image of a duplex stainless-steel weld, taken during the synchrotron experiments, is shown in the [figure on the right on p. 9](#).

Further analysis of the data available in the diffraction patterns allowed the team to determine the amount of ferrite and austenite present at each location. The top figure below shows the variation in the ferrite volume fraction as a function of location around the

weld pool. This is the first time the phenomenon was observed and quantified.

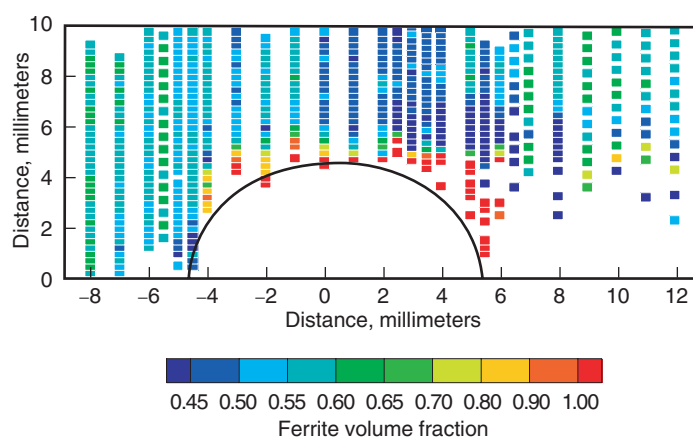
Once again demonstrating its unique capabilities, the SRXRD technique allowed the team to observe a decrease in the ferrite volume fraction at rather large distances from the weld pool (on the order of 9 millimeters). This change in the ferrite volume fraction was unexpected and had not been previously observed. Because evidence for this reaction disappears as the welding process continues, SRXRD provides the sole means available for monitoring these phase transformations.

### Research Leads to Smarter Welds

This pioneering work is not going unnoticed by the welding research community. Elmer was named a Fellow of the American Welding Society in 2000. And in May 2001, the society honored a paper by Elmer, Wong, and colleagues at Penn State with the prestigious William Spraragen Memorial Award. Their article on modeling of titanium welding was selected the best paper of 2000 in the *Welding Journal Research Supplement*.

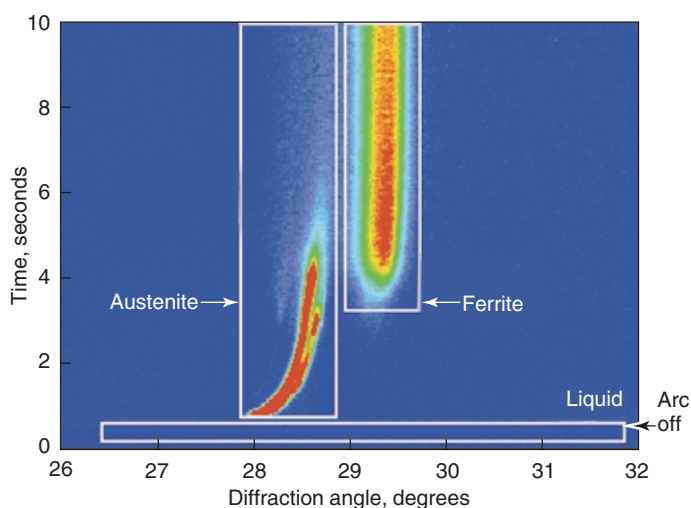
The ultimate purpose of all research on welding is to move useful information out to the welders of the world, to help them make better welds. In fact, Livermore synchrotron investigations of welds, combined with computer modeling and postweld characterization of microstructure, are beginning to do just that.

Powdered filler metal additions, which include aluminum, in flux-cored arc-welding electrodes alter the microstructure and properties of the resulting welds in unpredictable and undesirable ways. In the [bottom figure at the left](#), TRXRD results



Results of a spatially resolved x-ray diffraction experiment portray the dominant phase transformations and the regions over which they occur in the heat-affected zone during welding of duplex stainless steel.

Time-resolved x-ray diffraction results show phase transformations during weld solidification and cooling of a flux-cored arc-welding electrode.





show phase transformations during the solidification and cooling of a weld in a mild steel consumable welding electrode. This figure comprises over 500 diffraction patterns, taken at the rate of 20 patterns per second, and indicates an unexpected nonequilibrium solidification of the weld.

Nonequilibrium solidification translates into a possible safety hazard for welded structures. To mitigate the hazard, this research, which is being done in collaboration with Oak Ridge National Laboratory, is now being used to help design new self-shielded welding electrodes with improved weld properties for safer building and bridge construction. You can't get much more useful than that.

—Katie Walter

**Key Words:** fusion welding, phase transformation, solidification kinetics, spatially resolved x-ray diffraction (SRXRD), stainless steel, synchrotron radiation, time-resolved x-ray diffraction (TRXRD), titanium, x-ray diffraction.

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## About the Scientists



JOHN ELMER received his B.S. and M.S. in metallurgical engineering from the Colorado School of Mines in 1979 and 1981, respectively, and his Sc.D. in metallurgy from the Massachusetts Institute of Technology in 1988. After working briefly at Lawrence Livermore in the early 1980s, he rejoined the Laboratory as a postdoctoral scientist in 1988 and was named group leader for Materials Joining in 1989, a position he continues to hold. The group is responsible for electron- and laser-beam welding, vacuum brazing, and diffusion bonding.

Elmer has written or cowritten over 60 technical papers on materials joining, metallurgy, rapid solidification, the interactions of high-energy-density beams and materials, and the kinetics of phase transformations under nonisothermal conditions. He is a member of the American Welding Society (AWS) and the American Society of Metals International. In 2000, he was made a fellow of AWS; in 1991 and 2000, he received the William Spraragen Award from AWS; and in 1995, he received the Professor Masubuchi-Shinsho Corporation Award from AWS.



JOE WONG received a B.Sc. in pure and applied chemistry in 1965 and a B.Sc. in physical chemistry in 1966 from the University of Tasmania, Australia. In 1970, he received his Ph.D. in physical chemistry from Purdue University, and in 1986, he received a D.Sc. from the University of Tasmania. In 1986, he joined Lawrence Livermore as a senior chemist.

Wong's primary research interests include glass science and materials science. He has also examined the chemical dynamics and phase transformation of various materials and processes using high-resolution electron microscopy, various kinds of spectroscopy, and novel synchrotron instrumentation. He has written or cowritten over 175 journal articles, holds 7 U.S. patents, and has received numerous prizes and awards, most recently (with John Elmer) the William Spraragen Memorial Award from the American Welding Society for the best paper published in *Welding Journal Research Supplement* in 2000.



# Probing the Subsurface with Electromagnetic Fields

*Lawrence Livermore researchers are helping to squeeze more oil from production fields*

**F**OR years, energy experts have been warning the U.S. about our increasing dependence on imported oil. Although this country has abundant oil reserves, oil companies usually recover only about 32 percent of the oil in a typical reservoir. That is, for every barrel of oil withdrawn from an oil field, two are left behind. Recovering all the oil discovered is impossible; however, increasing production levels is a constant goal. Extracting even a relatively small additional amount of oil is important to the nation's energy future.

Researchers at Department of Energy national laboratories such as Lawrence Livermore have been working with U.S. oil companies to improve enhanced oil recovery (EOR) technologies so that more oil can be extracted from domestic production fields. One standard EOR technique, called waterflooding, pumps water underground to wash out oil trapped in rocks. Another method sends steam down wells to heat the oil and drive it toward production wells. A promising EOR method is injecting carbon dioxide underground. With carbon dioxide flooding, as much as 25 percent additional oil could be extracted that is

not presently retrievable with traditional EOR methods.

With all of these methods, it is important to monitor the EOR operation underground so that field personnel can track the injected material over time to better position production wells for increased recovery. Also, because EOR operations can last for several years, oil companies can save money when high-resolution imaging reveals a problem early, such as a layer of rock that is preventing water or gas from flowing through a field.

A technique to view underground fluids and gases, called crosswell electromagnetic (EM) imaging, is a valuable tool for monitoring steamflooding and waterflooding. Because of its demonstrated success with these two standard EOR methods, crosswell EM imaging is being tested by Lawrence Livermore researchers as a potential method to track carbon dioxide injected underground for EOR. The research team's early success with mapping carbon dioxide injected into a central California oil field has prompted discussion of using the technology to monitor the underground sequestration (long-term storage) of carbon dioxide

from industrial operations to help the environment. Finally, the team has also demonstrated the technology's usefulness in geothermal well drilling and as a method to monitor toxic waste spills.

## Exploiting Resistivity Differences

Crosswell EM imaging takes advantage of the differences in how electromagnetic fields are induced within various materials. (See the [box on p. 14.](#)) Rocks containing a lot of water, for example, usually conduct electricity better than rocks containing oil, typically in the form of droplets bound to tiny rock pores. EM imaging is complementary to traditional seismic imaging, which uses sound waves to visualize underground geologic strata. Seismic imaging, however, has limited capability to distinguish between oil and other fluids. "Seismic methods are best for mapping structure, while electromagnetic methods are sensitive to the types of fluids within rocks," says Lawrence Livermore physicist and lead researcher Barry Kirkendall.

Over the past several years, Livermore researchers have been improving the capability of crosswell EM imaging to map underground



waterfloods. Field experiments have demonstrated the technology at the University of California's Richmond Field Station in the San Francisco Bay Area and the Lost Hills oil field operated by Chevron USA in central California.

The successful imaging from the Lost Hills project prompted a new study to determine the usefulness of the technique for monitoring carbon dioxide flooding at a nearby site also operated by Chevron. The new study, begun last year, is funded by Laboratory Directed Research and Development in partnership with Chevron USA. The study combines both field work and laboratory experiments.

Kirkendall says that interest in using carbon dioxide as an EOR technique is increasing because its oil recovery rate can be higher than that of waterflooding or steamflooding. Pumping carbon gas or liquid carbon dioxide deep into the ground is done with a set of injection wells. The carbon dioxide remains in liquid form if it is injected deeper than about 550 meters. Above that level, the lower pressure turns the liquid into a gas. Liquid carbon dioxide has a bit more miscibility to drive oil from rocks than does gaseous carbon dioxide, but both phases are useful to oil recovery efforts.

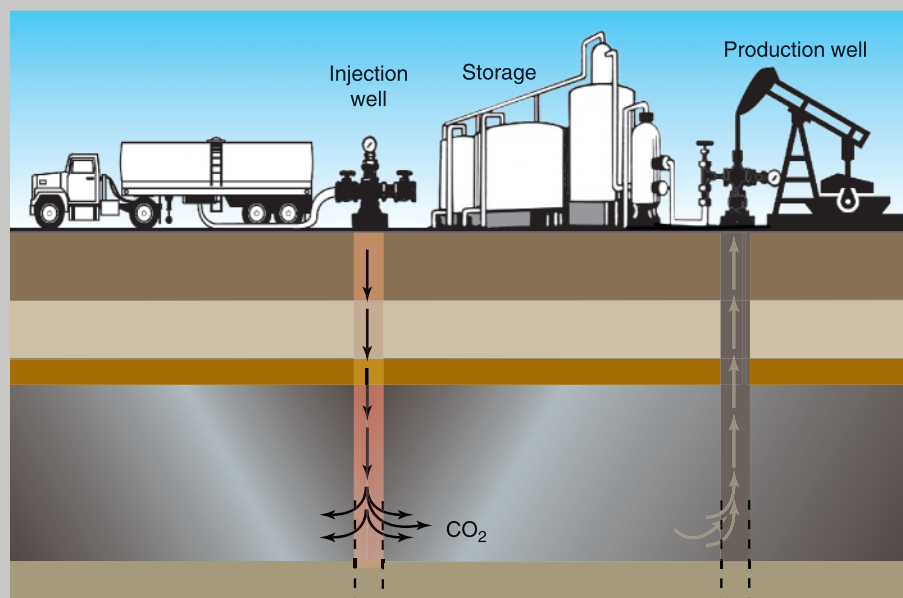
Underground, carbon dioxide travels slowly through rock layers, mixing with oil droplets in rock pores, lowering the droplets' viscosity, and thereby easing their extraction by production wells. When the now thinner oil reaches the surface, about 10 percent of the carbon dioxide comes out with the oil; the remaining 90 percent remains below ground. A good deal of water is also extracted with the oil and is separated and pumped back into the earth.

### Test at Lost Hills

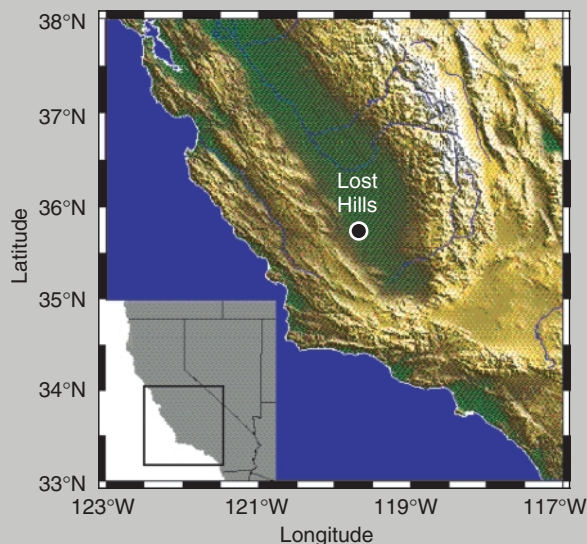
The current Lost Hills project tests the ability of crosswell EM imaging to map the location of carbon dioxide and remaining from a previous, multiyear waterflood. The study uses Lawrence Livermore field equipment

from the first Lost Hills for characterizing a waterflood. The equipment includes two new field vehicles that were obtained from DOE's Nevada Test Site. One vehicle is outfitted for signal transmission and the other for signal reception and data processing.

Kirkendall says that the Lost Hills project is especially valuable because the team obtained images of the underground environment in August 2000, some four months before Chevron began to inject carbon dioxide. These baseline images were acquired for comparison while tracking carbon dioxide, oil, and water



To enhance oil recovery, carbon dioxide (CO<sub>2</sub>) is pumped underground, where it mixes with oil, lowering the oil's viscosity and thereby improving the extraction by production wells. About 10 percent of the carbon dioxide comes out with the extracted oil. A good deal of water from previous waterflooding is also extracted with the oil.



The tests for crosswell electromagnetic imaging have been conducted mostly at the Lost Hills oil field in central California. The field is operated by Chevron USA.

over time. In April 2001, the researchers acquired subsurface data for comparison to the baseline, preinjection images. In October 2001, a six-month snapshot was taken. Additional data will be acquired in March 2002.

To acquire data, the team uses two fiberglass-cased observation wells located some 30 meters apart. One of four carbon dioxide injectors is located directly between the observation wells. A receiver is sent down one well and a transmitter is placed down the second. Each tool is connected by wire to its

respective field vehicle. The vehicles, in turn, are connected by fiber-optic cable. Data are acquired at three frequencies—2, 4, and 10 kilohertz—over the 92-meter depth interval between 455 and 550 meters, the depth at which carbon dioxide was injected.

Following extensive computer processing, the data recorded in April yielded images in the two-dimensional plane between the transmitter and receiver wells. The images show that carbon dioxide is slowly moving through the field, mixing with oil

droplets, and pushing them to production wells. However, the images also show that carbon dioxide is trapped in certain places instead of getting dispersed throughout the area. “The tests suggest that crosswell EM has the ability to characterize carbon dioxide displacement from water and oil in underground rock strata,” says Kirkendall.

### Laboratory Work Aids Effort

The team is working to better discriminate carbon dioxide from oil, a major task because both have similar

## Crosswell EM Imaging on the Job

Crosswell electromagnetic (EM) induction imaging technology was developed by researchers at Lawrence Livermore and Lawrence Berkeley national laboratories and scientists at Schlumberger, a supplier of oil production services (see *S&TR*, August 1996, pp. 20–23). The technology is designed to provide high-resolution images of underground deposits of oil, water, gas, and other materials. It was originally developed to provide oil companies with a means to monitor oil recovery techniques such as waterflooding. The technology is currently being tested for carbon dioxide flooding, a form of enhanced oil recovery, and for monitoring toxic spills.

Crosswell EM imaging is a complementary technique to traditional seismic imaging, which involves sending sound waves through underground geologic formations and investigating the different speeds at which the waves travel. Instead of measuring sound-wave velocities, the method measures electrical resistivity—or conversely, conductivity—of different materials to electromagnetic fields and waves. For example, rock formations containing water conduct current much more readily, that is, have a lower resistance, than rocks containing oil and gas. Injecting a field with steam or water—two common methods for forcing more oil out of rocks—lowers the resistivity of the rock. Images taken before, during, and after injection are compared to determine the progress of this enhanced recovery process.

Measuring electrical resistivity near a well is a longstanding technique in oil exploration and mapping geologic strata. Such measurements are usually made out to about a meter around the well. Crosswell EM induction permits mapping subsurface resistivity at multiple frequencies between wells to yield a detailed, two-dimensional picture.

The system consists of a transmitter tool deployed in one well and a receiver tool deployed in a second well, typically 30 meters away. The tools are connected to specially designed field vehicles obtained last year from the Department of Energy’s Nevada Test Site. The

transmitter uses a vertical axis coil wrapped with 100 to 300 turns of wire tuned to broadcast a single frequency that induces currents to flow in underground surrounding rocks. The induced current, in turn, generates a second magnetic field. At the receiver well, a custom-designed sensor detects the total magnetic field, consisting of the magnetic field from the induced currents as well as the primary magnetic field generated by the transmitter. A commercial lock-in amplifier, located in the receiver vehicle, extracts signals that are coherent with the transmitted signal while rejecting all noise.

In practice, the receiver is held steady at a fixed depth while the transmitter is lowered over the entire vertical length of the underground zone of interest. Then the receiver is held steady at a fixed depth, and the receiver is moved up and down. By positioning both the transmitter and receiver tools at various depths within the zone of interest, researchers create an image of the resistivity distribution for the geologic strata between the wells.

The entire process is done at two and, increasingly, three different frequencies (2 kilohertz, 4 kilohertz, and 10 kilohertz), because each frequency yields additional information. Lower frequencies give greater penetration through the subterranean rock layers, while higher frequencies give greater resolution. The transmitting frequencies are chosen based on the distance between the transmitting and receiving wells, resistivity measurements of the field taken by Chevron USA, and the unique characteristics of the rock layers based on laboratory work on the core samples.

An inversion algorithm developed at Sandia National Laboratories processes the collected data, essentially voluminous measurements of magnetic fields. The method is called inversion processing because magnetic field data of varying amplitude and phase are changed to electrical conductivity data corresponding to depth and distance between the transmitter and receiver wells. It takes several weeks to



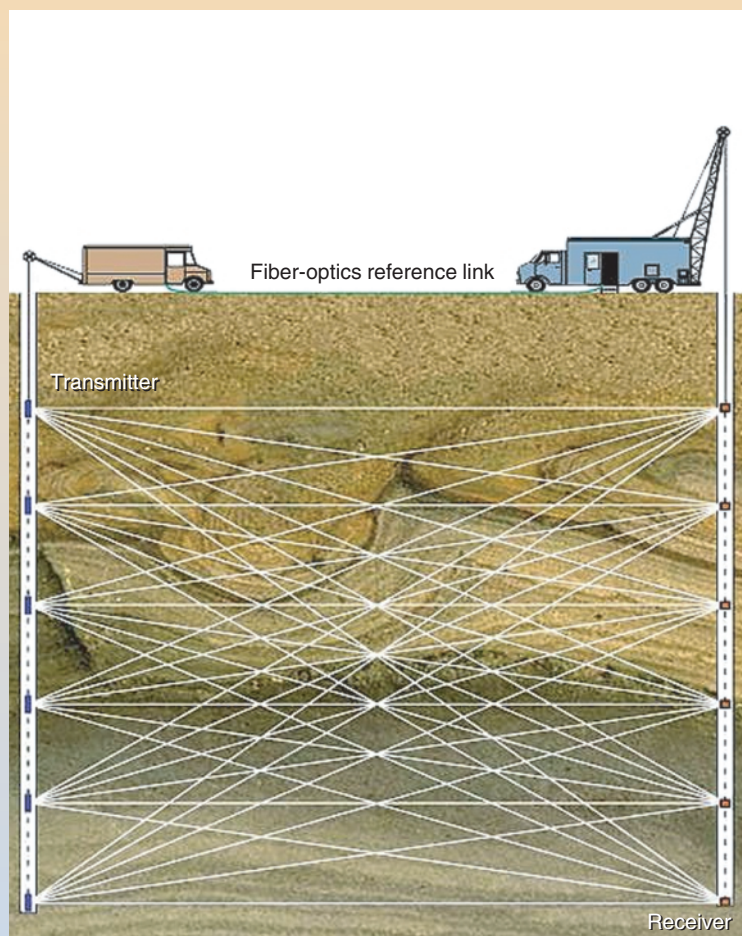


At the Lost Hills oil field, the receiver truck has lowered the underground sensor deep into the receiver well to detect the electromagnetic currents given off by the transmitter tool. The truck contains equipment for signal reception and data processing. Lawrence Livermore technicians Duane Smith (left) and Pat Lewis stand by the truck.

completely process all the data and build several possible underground computer models. Choosing the best model is aided by the results from laboratory tests on core samples from the field and from subsurface data obtained by the oil company working that field.

An outgrowth of the separate receiver and transmitter configuration is a single tool containing a transmitter located on top of several receivers arrayed vertically. This technique was used last year in a venture between Lawrence Livermore researchers, Schlumberger, and the California Energy Commission at several sites in California and Nevada. The technique looks in 360 degrees around an observation well and can take measurements some 10 meters into the formation.

Crosswell electromagnetic induction uses a transmitter tool deployed in one well and a receiver tool deployed in a second well. The tools are connected to specially designed field vehicles. The transmitter broadcasts a frequency that induces currents to flow in underground surrounding rocks. The induced current, in turn, generates a second magnetic field. At the receiver well, a sensor detects the magnetic fields. The receiver is held steady at a fixed depth while the transmitter is lowered over the entire vertical length of the underground zone of interest. Then the receiver is held steady at a fixed depth and the receiver is moved up and down. In this way, researchers create an image of the resistivity of the geologic strata located between the transmitter and receiver.



electrical signatures. In addition, Kirkendall relies on experimental data supplied by Livermore geophysicist Jeff Roberts. Working in his laboratory, Roberts measures the electrical properties of core samples taken from deep underground by Chevron engineers. The experiments determine the electrical properties of the production field's rocks as they are saturated with fluids and carbon dioxide.

Roberts had conducted similar experiments on core samples from the Lost Hills waterflood study, but he had to modify some procedures and techniques so that he could use carbon dioxide as an injectate. The current experimental setup consists of a heated pressure vessel capable of confining pressures up to 10 megapascals and temperatures up to 300°C. Roberts takes well-characterized water- and oil-saturated samples and forces carbon dioxide into them, driving oil out in the process. He records the

sample's changing electrical properties as the oil is pushed out. Next, he lowers the pressure so that the liquid carbon dioxide changes to the gas phase, and he monitors the electrical changes.

A second type of experiment involves injecting gaseous carbon dioxide and monitoring the electrical properties. All of the experiments are repeated at the different transmitting frequencies that are used in the field.

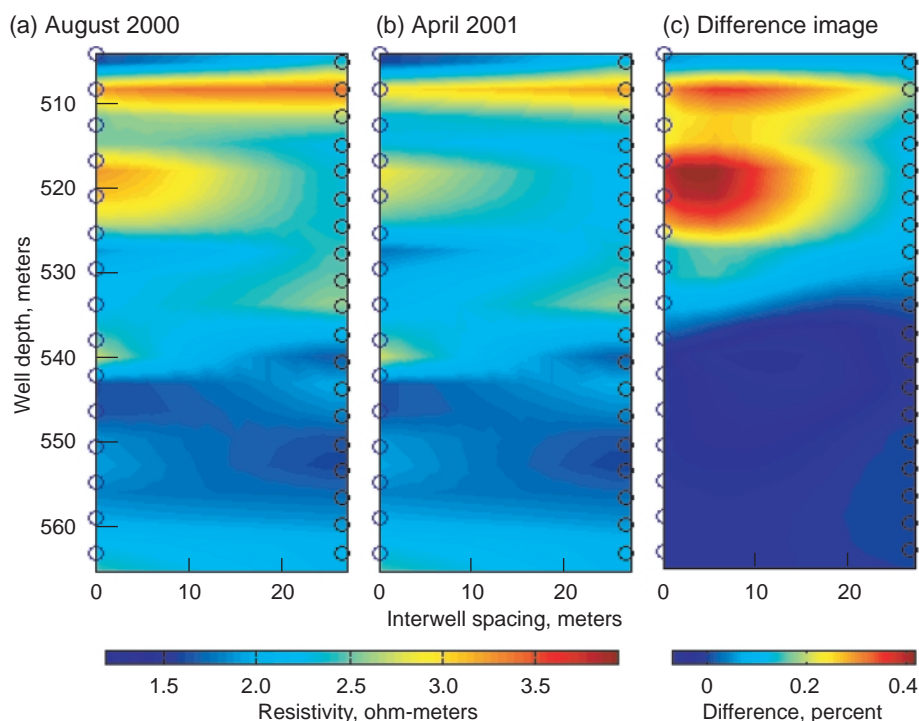
Roberts notes that samples undergoing carbon dioxide invasion may change geochemically. The nature of the geochemical change depends on such factors as rock chemistry and mineralogy, temperature, pressure, and the chemistry of the fluids inside the rock pores. These changes can affect measured electrical properties. The laboratory data thus help to interpret the EM field data more accurately by improving the resolution between carbon dioxide and oil, which have

similar electrical conductivities. "This kind of laboratory work is critical to getting the most information out of the field measurements," says Roberts.

Kirkendall notes that Lost Hills contained an estimated 9 billion barrels of oil. However, after decades of oil production, only 9 percent of the oil has been recovered, because Lost Hills oil is typical California crude—thick and heavy and therefore difficult to pump out of the ground. As a result, 55 percent of the oil currently produced in California comes from EOR methods. At Lost Hills, these methods include hydrofracturing, or breaking up rock layers to create additional pathways for oil to travel, and longer-term waterfloods and steamfloods to sweep trapped oil to the producing wells.

While carbon dioxide injection for EOR provides higher yields than other recovery methods, it is much more expensive than waterflooding. "Water

Two-dimensional images of carbon dioxide flooding in the plane between the two observation wells—one for transmitting, the other for receiving. Image (a) was generated before injection of carbon dioxide and after waterflooding, and image (b) was generated after 3 months of injection. The circles on the left side of each image represent the wells containing the receiver antenna, and the circles on the right side of the images represent the wells containing the transmitting antenna. (c) The difference image is the preinjection image subtracted from the during-injection image and shows areas of change quite clearly. A positive percent difference suggests carbon dioxide is entering the area at the top left. Blue represents water in place, and yellow and red represent the moving oil and carbon dioxide, respectively. Laboratory work is helping to suggest which area is oil and which is carbon dioxide.



flooding is cheap because it can usually be done with brackish water that's available on site," says Kirkendall. As a result, carbon dioxide flooding, if adopted by the industry, would be done only after waterflooding or steamflooding and would be followed by additional waterfloods or steamfloods.

Carbon dioxide flooding is being explored as an option for extending oil production in other states including Kansas and Alaska. Experts estimate that between 2006 and 2010, oil recovered from increasingly depleted Alaskan fields will be too thick to flow in the Alaska pipeline. Injecting water or steam underground would melt the permafrost and collapse wells, so using carbon dioxide might be the best solution.

Bringing in trucks carrying liquid carbon dioxide accounts for most of the expense associated with carbon dioxide flooding. But, Kirkendall maintains, "If a pipeline furnished carbon dioxide

gas to an EOR site, costs would be dramatically reduced. The idea of building carbon dioxide pipelines has intrigued energy and environmental scientists because power plants and factories produce large amounts of the gas. If the carbon dioxide were to be captured at the smokestack, it could be transported by pipeline to an oil production field for enhanced production."

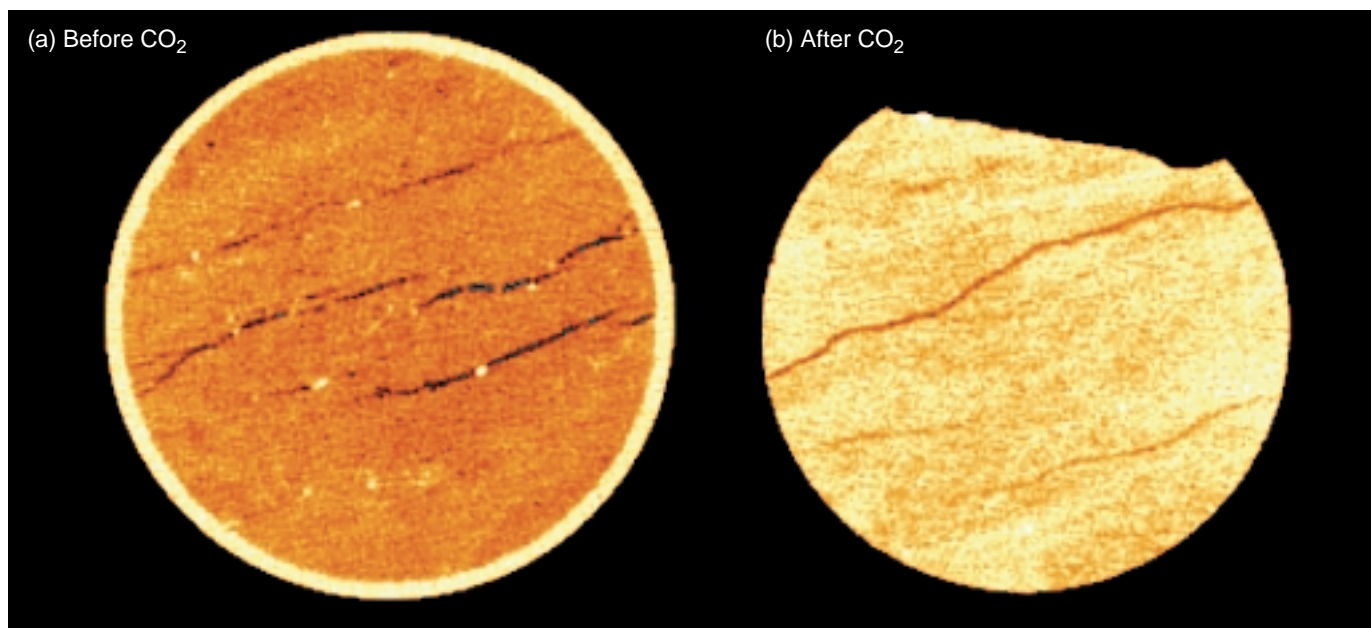
Kirkendall notes that several new natural-gas-fired power plants were recently approved for California's San Joaquin Valley, close to Lost Hills. The carbon dioxide output of the power plants could be transported to the site by pipeline and injected into the subsurface to assist in EOR, all at a small fraction of the price for trucking in liquefied carbon dioxide. Crosswell EM imaging could then be used to map the carbon dioxide during initial injection. For the highest cost savings, permanent

underground electromagnetic transmitters and sensors would be used for long-term monitoring.

### Storing CO<sub>2</sub> for the Environment

Apart from enhanced oil recovery, injecting carbon dioxide underground for long-term storage could become an important way to remove excess amounts from the atmosphere. Carbon dioxide is one of several greenhouse gases that have been linked to rising global temperatures. Significant amounts of carbon dioxide could be removed at the smokestack and then sequestered underground in oil fields and elsewhere instead of released to the atmosphere.

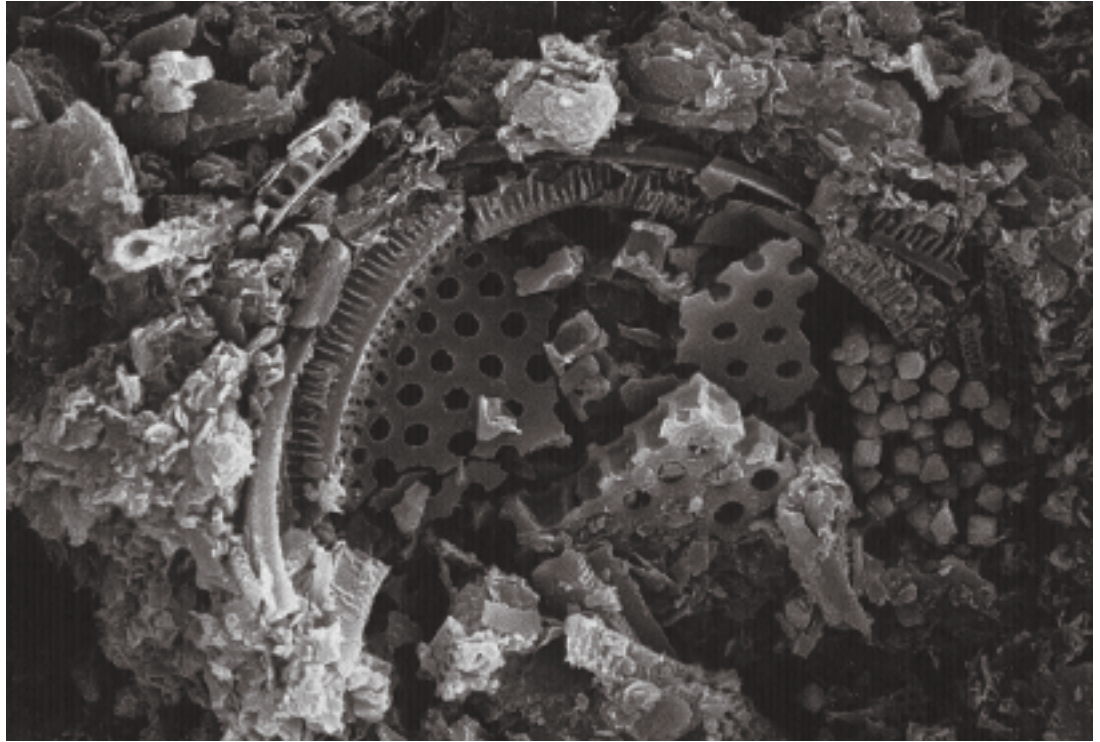
The federal government is considering carbon sequestration as part of its strategy for addressing climate change concerns. "Carbon sequestration is an important option to study because it offers a way to address the global



X-ray images of 5-centimeter-diameter core samples taken from the Lost Hills oil field show the effectiveness of carbon dioxide (CO<sub>2</sub>) to sweep oil. (a) A core sample before oil and then carbon dioxide are injected into the sample; (b) the sample after carbon dioxide injection, showing very little oil remaining.



A Chevron scanning electron micrograph reveals what makes extracting oil from the Lost Hills field a challenge: highly porous, low-permeability geologic strata filled with the silica skeletons of microscopic sea creatures, or diatoms (center), and crystals of the mineral pyrite (cubes at center right). (Courtesy of Mike Morea, Chevron USA.)



warming issue without having to make radical overhaul of our existing energy systems,” Energy Secretary Spencer Abraham said in July 2001. The Department of Energy’s Office of Fossil Energy, which oversees sequestration research, has set a goal of developing carbon dioxide sequestration options that cost \$10 or less per ton of carbon, equivalent to adding only 0.2 cents per kilowatt-hour to the average cost of electricity.

As with using carbon dioxide for EOR, sequestering carbon dioxide to help mitigate global warming would require some way to determine its location over time. “Crosswell EM imaging could ensure sequestered carbon dioxide is not leaking back into the atmosphere,” says Kirkendall.

The team will continue to monitor the carbon dioxide flood site for

another 12 months. Part of that effort will be continuing the laboratory experiments on core samples supplied by Chevron and focusing on ways to more clearly distinguish between carbon dioxide and oil.

Kirkendall presented the initial results from Lost Hills at the DOE’s National Energy Technology Laboratory’s first annual carbon sequestration conference in Washington, D.C., in May 2001. The response from scientists, representing both research centers and oil companies, was highly enthusiastic.

### Extending the Applications

“The techniques we’ve developed for EOR and carbon sequestration can be extended to several other applications,” Kirkendall says. For example, in August, the team visited DOE’s

complex at Hanford, Washington, the nation’s largest environmental cleanup site. The Livermore researchers are studying the use of the technology for tracking the radioactive wastes that are stored in Hanford’s underground tanks, the legacy of decades of plutonium production.

The team is also working with Schlumberger and the California Energy Commission to use single-well EM imaging to help guide the location of new geothermal wells. In August, Roberts made a presentation on the geothermal work to the Geothermal Resources Council, a professional organization. Kirkendall says the technology could also be applicable to natural gas reservoir monitoring.

One major challenge is modifying the imaging process so that it works better with wells encased in steel.



Often, sites have one fiberglass well for monitoring, and the remainder are cased in carbon steel, a material that significantly weakens EM signals. As a result, the potential commercial application of crosswell EM imaging depends on how well the procedures and modeling codes handle electromagnetic transmission through steel casing. In the studies at Lost Hills, both the transmitter and receiver wells are fiberglass.

Another task includes developing permanent, inexpensive sensors for long-term monitoring at much lower costs. Permanent underground sensors are a particularly attractive option for long-term carbon dioxide sequestration. Based on the results so far, the imaging team is confident crosswell EM imaging has a strong future in the nation's energy and environmental future.

—Arnie Heller

**Key Words:** carbon sequestration, crosswell electromagnetic (EM) imaging, enhanced oil recovery (EOR), oil production.

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## About the Scientists



**BARRY KIRKENDALL** received a B.Sc. in physics from the University of California at San Diego in 1992 and an M.Sc. in geophysics from the Colorado School of Mines in 1998. Before joining the Laboratory, he was a staff research assistant at the Scripps Institute of Oceanography in La Jolla, California, with a focus on ocean-bottom seismology, and an electrical engineer at Caterpillar Research Facility in Illinois, where he was involved in the development of a ground-penetrating radar system for rapid near-field imaging. He came to Livermore in 1998 as a physicist responsible for managing a project to develop cross- and single-well electromagnetic subsurface imaging and associated data-acquisition systems. Current projects include near-surface high-frequency three-dimensional imaging, multiple frequency imaging at oil and gas sites, and near-wellbore imaging of fracture systems at geothermal sites. The emphasis of this research is on using electromagnetic induction imaging coupled with petrophysical research to monitor enhanced oil recovery through carbon dioxide injection and sequestration. Kirkendall is the principal investigator responsible for field studies for this enhanced oil recovery research at Livermore.



**JEFF ROBERTS** came to the Laboratory in 1992 as a geophysicist. He received his B.S. in applied science from the University of Texas at San Antonio in 1985 and his Ph.D. in geology from Arizona State University in 1992. His primary research interests include the electrical properties of minerals and rocks, the physics of flow and transport, the physical properties of porous media, and the microscale imaging of materials to reveal flow and transport. He also researches solid-earth geophysics, particularly the experimental determination of the physical properties of rocks and minerals, with the goal of more fully understanding the composition and dynamics of Earth's interior. He is the coauthor of numerous journal articles on these topics. He is currently the principal investigator responsible for laboratory experiments on Livermore's project using electromagnetic induction imaging to monitor enhanced oil recovery through carbon dioxide injection and sequestration.



# Probing the Liquid Water Surface

**W**ATER. It covers 70 percent of Earth's surface, makes up 60 percent of the human body, and forms 90 percent of the composition of blood. Life as we know it wouldn't exist without water. Yet, each molecule of this common, seemingly simple substance—one oxygen atom bound to two hydrogen atoms—holds a world of mystery within its subnanometer-size structure.

Of particular interest to physical and structural chemists is what happens at the interfaces where water meets air or other substances such as proteins. The density of the water molecules, for example, can change by many orders of magnitude between the liquid below the surface and the vapor above the surface. What happens in the transition zone? Much has been theorized and calculated, but corroborating experiments have been difficult to conduct—until now.

A team of researchers from Lawrence Livermore and Lawrence Berkeley national laboratories and the University of California at Berkeley has developed a technique using soft x rays for studying in detail the surfaces of liquid microjets. The groundbreaking work of the collaboration, which included Livermore chemist James Tobin, UC Berkeley chemistry graduate student Kevin Wilson, and UC Berkeley chemistry professor Richard Saykally, was reported in both *Physical Review Letters* and a cover article in the *Journal of Physical Chemistry B*.

The standard technique for examining the chemical structure of a protein at the molecular and atomic levels, for example, uses a frozen sample. Yet, the three-dimensional structure of molecules in a frozen sample differs from that of molecules in a sample at body temperature. "There's a strong drive to find ways of studying the molecular structures of such substances in their normal biological state," explains Tobin. "The experimental technique we developed is one possible method." Ultimately, this technique may allow scientists to better determine the structure of biological systems such as hemoglobin in blood and to understand how proteins move through solution.

## X Rays Measure Atomic Interfaces at Water's Surface

One of the primary tools for probing the electronic structure of interfaces is x-ray absorption spectroscopy. However, this x-ray technique has difficulty measuring the structural interfaces at the atomic and molecular level for liquids, particularly those containing hydrogen atoms. "And hydrogen is a key atomic component in many systems," says Wilson. "Many of the interesting properties of water are due to the hydrogen bonds between neighboring molecules." (See the [box on p. 21.](#))

One problem facing scientists who want to examine hydrogen's role in water or other liquids is that the amount of spectroscopic data gathered from hydrogen on the surface or interior of a water sample is extremely small. This weak signal is usually overwhelmed by signals generated from the water vapor that blankets the surface of liquid. Another problem is that with x-ray spectroscopy systems, the sample must be in a vacuum, which means the liquid must be contained or behind a barrier such as a window. "Windows, even thin-walled cells, will interact with the surface of the liquid and absorb a majority of the x-ray signal, leaving us nothing to measure by," Tobin explains.



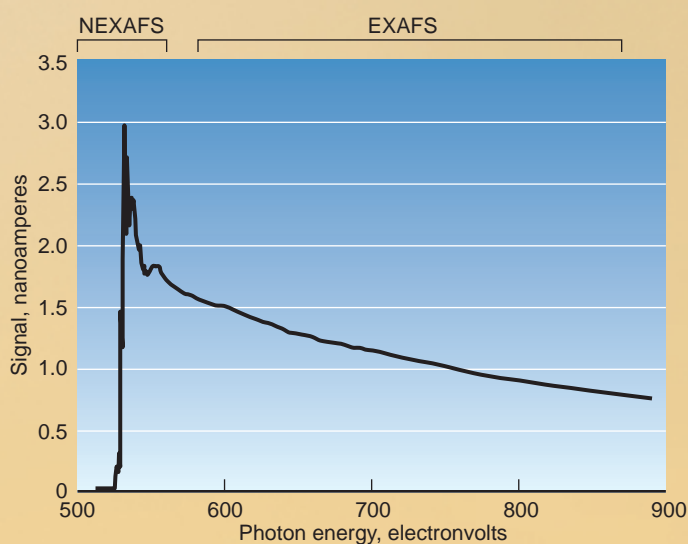
The team overcame these problems, using liquid microjet technology and Lawrence Berkeley's Advanced Light Source (ALS). In the experiments, a 20-micrometer-diameter jet of liquid pressurized to about 3.4 megapascals (500 pounds per square inch) squirts through a very small nozzle. "The smaller the dimensions of a liquid sample, the less vapor there is," explains Wilson. Two other team members, Lawrence Berkeley beamline scientists Bruce Rude and Tony Catalano, devised a pumping system that not only allowed the system to meet the vacuum requirements of the ALS but also reduced the amount of residual vapor. "As far as I know, these experiments were the first time that experiments on a liquid jet were conducted at the ALS," notes Wilson.

To probe the structure of water molecules at the surface of the water jet, researchers use intense x-ray beams of energies at the "soft" end of the spectrum generated by the ALS. The x rays are directed at the jet about 1 to 2 millimeters in front of the nozzle. At this distance, the liquid is still at room temperature and has not yet begun to expand and cool. Because it is impossible to examine anything smaller than the wavelength of light being used, the light waves for studying atoms and molecules must be extremely short. The ALS is ideal for these sorts of measurements, because it can produce light at wavelengths of a few tenths of a nanometer—about the sizes of atoms, molecules, chemical bonds, and the distances between

atomic planes in crystals. Even more importantly, the ALS can supply x rays at 530 electronvolts and above—the amount required to "kick" an electron from the innermost shell of an oxygen atom out of the water molecule. (See the [box on p. 22](#).)

### Electrons at the Edge

Two x-ray spectroscopy techniques were used to examine the structure of the water surface in the microjet: extended x-ray absorption fine structure (EXAFS) and near-edge x-ray absorption fine structure (NEXAFS). Both techniques are based on the fact that atoms will absorb x rays, the amount of absorption depending on the energy level of the x ray and the type of atom doing the absorbing. Generally, the proportion of x rays absorbed (called the absorption coefficient) decreases as x-ray energies increase. However, at energy levels specific to each element, a sudden increase in the absorption coefficient is observed. These energies, called absorption edges, correspond to the energy required to eject an electron



X-ray absorption spectra at the oxygen K edge (530 electronvolts) of water vapor showing the near-edge x-ray absorption-fine-structure (NEXAFS) and extended x-ray absorption-fine-structure (EXAFS) regions of the spectra.

### Water Basics

Water is the most familiar and abundant liquid on Earth. Given its low molecular weight, it should, by all rights, be a gas at such temperatures. The fact that it is not has much to do with its molecular structure. The atoms in a water molecule—two hydrogen and one oxygen—are arranged at the corners of an isosceles triangle. The oxygen atom is located where the two equal sides meet, and the angle between these sides is about 105 degrees. The asymmetrical shape of the molecule arises from a tendency of the four electron pairs in the outermost shell of oxygen to arrange themselves symmetrically at the vertices of a tetrahedron around the oxygen nucleus. Two electron pairs from each oxygen form covalent bonds with the two hydrogen atoms. (A covalent bond is created when two atoms share a pair of electrons.) The hydrogen atoms are drawn slightly together, resulting in the V-shaped water molecule. This arrangement results in a polar molecule, with a net negative charge toward the oxygen end and a net positive charge at the hydrogen end. When water molecules are close enough, each oxygen attracts the nearby hydrogen atoms of two other water molecules, forming hydrogen bonds. Although much weaker than the covalent bonds holding the water molecule together, hydrogen bonds are strong enough to keep water liquid at ordinary temperatures, despite its low molecular weight. These hydrogen bonds are also responsible for various other properties of water, such as its high specific heat.



from the atom. For an isolated atom, the sudden peak at the absorption edge occurs as the electron is ejected and then a gradual decrease in x rays absorbed occurs as the x-ray energy levels are increased. However, for atoms in a molecule or in a liquid or solid state, the closeness of other atoms around the absorbing atom causes oscillations in the amount of x-ray absorption just past the absorption edge. These “wiggles” detected in the absorption edge, called EXAFS oscillations, arise from the ejected electron backscattering off neighboring atoms. The structure of the oscillations—that is, their frequency and amplitude—depends on the distance and number of neighboring atoms. The length of bonds between neighboring atoms—such as oxygen atoms or hydrogen atoms in water, for instance—can be determined by analyzing these EXAFS oscillations.

Whereas EXAFS is sensitive to distances between atoms and molecules, NEXAFS is sensitive to bond angles and bond lengths between atoms and molecules. NEXAFS is similar to EXAFS, but instead of providing enough energy to eject an electron, a NEXAFS x ray has just enough energy to cause an electron to jump up to an unoccupied higher energy level. The steplike vertical rise in absorption intensity resides between

the absorption edge and the EXAFS region, hence the “near-edge” designation. The energy at which this rise occurs differs according to the individual element, chemical bond, or molecular orientation. With NEXAFS, researchers tune the x-radiation to different frequencies to help determine the orientation of a molecule on the surface of a liquid and its intramolecular bond lengths.

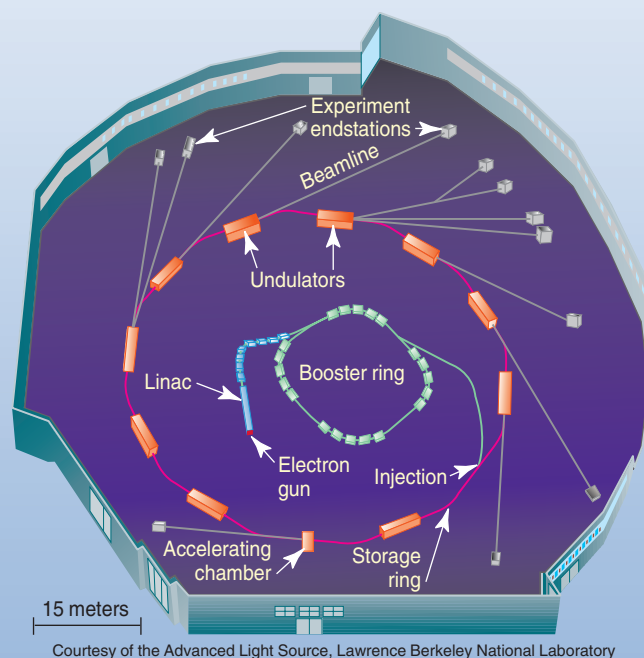
### Measuring the Ties That Bind

In their first experiment, reported in *Physical Review Letters*,<sup>1</sup> the team members made the first definitive observation of EXAFS from hydrogen and quantified the covalent oxygen–hydrogen bond in water vapor as  $0.095 \pm 0.003$  nanometer in length. Their research showed that hydrogen bonds can be directly detected in liquid water, paving the way for future studies of intermolecular hydrogen bonds—structures that are critical to understanding the unique properties of liquid water.

In their second experiment, reported in *The Journal of Physical Chemistry B*,<sup>2</sup> the researchers obtained NEXAFS spectra for the water surface that appear as intermediate between the bulk- and the gas-phase spectra. The appearance

## How the ALS Works

The Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory generates intense light for scientific and technological research. As the world’s brightest source of ultraviolet and soft x-ray beams and the world’s first third-generation synchrotron light source in its energy range, the ALS makes previously impossible studies a reality. Inside the ring structure of the facility, electrons traveling at nearly the speed of light are forced into a circular path by magnets and emit bright ultraviolet and x-ray light that shines down beamlines to experiment stations at the end of the lines. The x-ray light produced is one billion times brighter than the Sun’s. This high brightness means that the x rays are highly concentrated, allowing many x-ray photons per second to be directed onto a tiny area of a material. The increased illumination allows one to “see” in more detail, just as seeing details in a landscape is easier at noon, when there are many photons from the Sun, rather than at dusk, when the photons are fewer. Researchers use the ALS for protein crystallography, ozone photochemistry, x-ray microscopy of biological samples, and optics testing as well as for studying the electronic structure of matter. For more information about the ALS, see [www-als.lbl.gov/](http://www-als.lbl.gov/).





of the surface spectrum is consistent with an interface or surface in which molecules are in transition from the bulk phase to the vapor phase as in evaporation. The researchers measured distances of  $0.3 \pm 0.005$  nanometer between neighboring oxygen atoms on the surface of the microjet, and distances of  $0.285 \pm 0.005$  nanometer between neighboring oxygen atoms about 2.5 nanometers inside the jet. The latter result is in line with previous studies of the bulk liquid. The surface measurement supports results from computer simulations, which predicted that on the surface, weaker hydrogen bonds would exist, leading to water molecules that would be further apart and more mobile compared to molecules below the surface.

“What these experiments showed was that this technique works and works well,” says Tobin. Since the results were published, the team has moved forward, using this technique to examine molecular structures of other solvents such as methanol, ethanol, and isopropyl alcohol. One of the next steps will be to examine sodium chloride solution—in other words, salt water. It’s all just the beginning of obtaining a better understanding of liquid surface chemistry—one of the big unknowns in modern science.

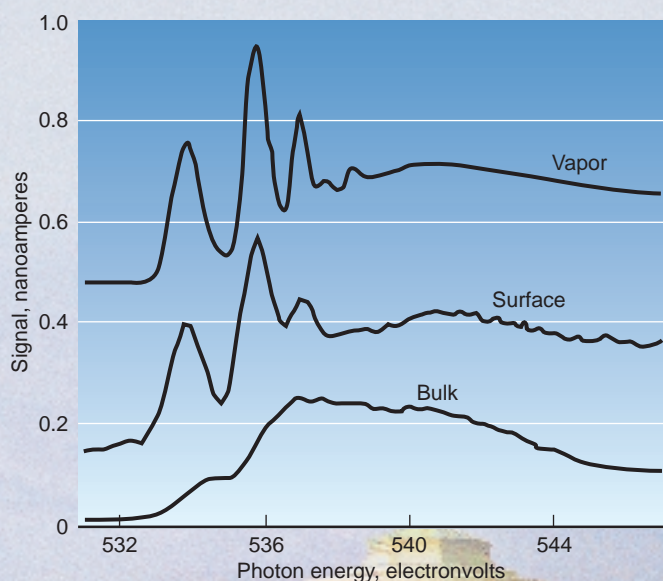
—Ann Parker

**Key Words:** Advanced Light Source (ALS), extended x-ray absorption fine structure (EXAFS), hydrogen bonds, liquid surface chemistry, microjet, molecular structure, near-edge x-ray absorption fine structure (NEXAFS), water, x-ray spectroscopy.

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2. Kevin R. Wilson, Bruce S. Rude, Tony Catalano, Richard D. Schaller, James G. Tobin, Dick T. Co, and R. J. Saykally, “X-Ray Spectroscopy of Liquid Water Microjets,” *The Journal of Physical Chemistry B* **105**(17), 3346–3349 (2001).  
[www.llnl.gov/str/refs/tobin.r2.html](http://www.llnl.gov/str/refs/tobin.r2.html)

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Near-edge x-ray absorption-fine-structure (NEXAFS) spectra of water vapor (top), liquid water surface (middle), and bulk, or interior, water (bottom), showing the surface to have an intermediate electronic structure between vapor and the bulk liquid.

Courtesy of the Advanced Light Source, Lawrence Berkeley National Laboratory



## New Targets for Inertial Fusion

**A** central goal of fusion energy research is to develop the technology and firm scientific understanding to warrant construction of an electric power plant. One route to commercial fusion energy is inertial fusion, and a leading means of creating inertial fusion is with high-energy lasers. In this technique, laser pulses either directly compress a BB-sized capsule, or target, of fusion fuel (deuterium and tritium ions), causing the fuel to ignite; or the pulses are converted first into x rays inside a metal case, called a hohlraum, that contains the fuel capsule, and the x rays compress the capsule, leading to ignition of the fuel. The first method is called direct drive, and the second is termed indirect drive. In both methods, the goal is to have the fuel maintain compression long enough for its

deuterium and tritium nuclei to fuse and liberate more energy than is required to drive the reaction. The ratio of energy in to energy out is called gain. The energy produced will be used to boil water to drive the electric turbines of a commercial power plant.

In practice, however, achieving inertial fusion requires enormous energy delivered uniformly to the capsule. For years, scientists have explored ways to achieve inertial fusion that reduced the cost and are compatible with a power plant. Two concepts—heavy-ion fusion and fast ignition—are being explored by Lawrence Livermore physicists and collaborators as attractive candidates for producing commercial electricity through fusion.

A team of Lawrence Livermore physicists led by Max Tabak is exploring target designs for both concepts as part of the Department of Energy's Inertial Fusion Energy Program. Tabak notes that the feasibility of an inertial fusion energy power plant is strongly affected by the requirements of the target for achieving ignition and high gain. "We want targets that will contribute to lower system costs," he says. That means targets that are easy to fabricate, that minimize environmental hazards produced during the fusion reaction, and that permit higher energy gains.

### Using Heavy Ions Instead of Photons

The heavy-ion-fusion concept, first discussed in 1975, replaces lasers with induction accelerators that produce intense beams of heavy ions such as lead. Accelerators that produce ion beams for high-energy physics research have demonstrated 20- to 40-percent operating efficiency, as opposed to the 5- to 10-percent efficiency of lasers. The difference is important because driver efficiency determines how much of the electricity produced must be fed back to power the driver. In addition, scientists have ample experience using accelerators at about 10 hertz (repetitions per second). Scientists believe that 10 hertz, the approximate firing rate of a car engine at idle, is about the rate at which an accelerator would need to fire at an inertial fusion power plant.

"Heavy-ion beams are potentially a better means of carrying energy and power to a target than are the photons of

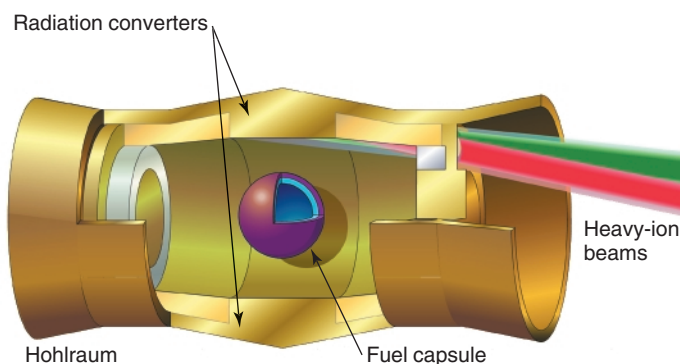
a laser,” Tabak says. Heavy ions are preferable to light ions because their current would be tens of kiloamperes lower. Lower beam currents make focusing the beam, done with magnetic fields, easier. In contrast, beams of protons, the lightest ions, would generate enormous currents that would be more difficult to focus.

However, scientists are unsure whether powerful ion beams could be focused easily onto targets. The problem is that unlike photons, which are electrically neutral, ions “feel” their electrical charge and, as a result, tend to move away from each other. This self-repulsion could make precise focusing difficult. “Heavy-ion beams present major scientific challenges,” says Tabak, “but many experts believe they are surmountable.”

The team is working on a broad range of target designs to satisfy both accelerator builders, who want designs that best couple the ion energy to the fusion fuel, and target builders, who desire designs that are cost-effective and easy to mass-produce. “We’re giving both groups a lot of options,” says Tabak.

### And the Leading Candidates Are . . .

The leading target candidates are so-called distributed radiator targets in which a metal hohlraum contains carefully located radiation converters to stop the ion beam and symmetrically convert its energy into x rays that compress and ignite a plastic fuel-filled capsule. One variant is a close-coupled target, designed by Lawrence Livermore physicist Debra Callahan-Miller, that features a smaller hohlraum. This design permits halving the heavy-ion beam energy required to



The leading target design for heavy-ion-beam fusion are so-called distributed radiator targets in which a metal hohlraum contains radiation converters to stop the ion beam and symmetrically convert its energy into x rays that compress and ignite a plastic capsule containing fusion fuel.

obtain fusion. However, the close-coupled target also requires a smaller beam focal spot than conventional distributed radiator targets. Simulations using Livermore’s LASNEX code show gains of 130 (energy liberated by the fusion reaction divided by energy put into the target) at 3.3 megajoules of ion beam energy and 90 at 1.75 megajoules of ion beam energy.

Another option is a hybrid design by Callahan-Miller that features a thick metal shield to block the path of the heavy-ion beam. The energy deposited behind the shield radiates through the hohlraum to the capsule. Because this design alone does not produce adequate symmetry of the fuel capsule, iron radiation shields are used to remove the last 1 to 2 percent of asymmetry.

The team’s heavy-ion target designs are part of a wider effort of the Lawrence Livermore Heavy Ion Fusion group that is working to understand better the physics of intense ion beams and their interactions with fusion targets. The group is a part of a national inertial fusion effort that includes fusion researchers at Lawrence Berkeley and Sandia national laboratories, Princeton Plasma Physics Laboratory, General Atomics, Massachusetts Institute of Technology, and other centers.

### Fast Ignition Adds Second Driver

Fast ignition was conceived by Tabak and other researchers in 1990. Since publication of the first paper in 1994, research on the concept has spread from Livermore to other national laboratories and to research centers in Europe, Japan, and Russia.

Fast ignition can be used with laser-driven direct or indirect drive, greatly relaxing the efficiency requirement on the driver and providing an attractive pathway to fusion energy. In fast ignition, the capsule’s deuterium–tritium fuel is first compressed to high density by a standard laser pulse lasting 1 to 10 nanoseconds. Then, an extremely short, 10- to 100-picosecond, high-intensity pulse from a second laser, presumably a petawatt laser, ignites the fuel’s dense plasma core with enormous currents (1 billion amperes) of super-hot electrons. (The first petawatt laser was developed by Lawrence Livermore researchers in the mid-1990s to test the fast ignition concept.

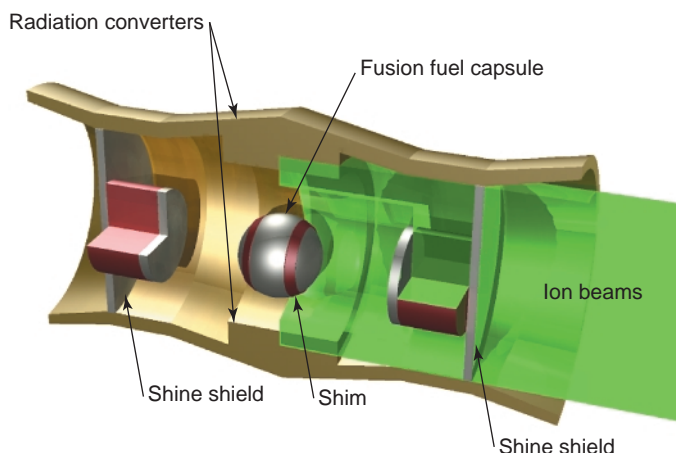
See *S&TR*, March 2000, pp. 4–12.) A hybrid fast-ignition concept has been explored in which target compression is accomplished with an ion beam and ignition is achieved with a petawatt laser.

Fast ignition offers the prospect of significantly reduced driver energy and the compression symmetry needed to achieve ignition. For example, various models show that the required energy of the compression beams could be reduced from 3 to 5 megajoules to less than 1 megajoule. Even with the added cost



of the ignition laser, such relaxed driver requirements might provide capital cost savings of 30 to 40 percent for a fusion power plant. Tabak says that fast ignition should also allow lower target-fabrication-finish requirements.

The Livermore team has also explored several different target geometries for fast ignition. Tabak notes that fast ignition may not need a hohlraum. The overriding design requirement is to ensure that the energy from the petawatt laser couples efficiently to the ignition region of the compressed fuel.



A hybrid design for heavy-ion beam fusion features a thick metal shield that blocks the path of the heavy-ion beam. The energy deposited behind the shield radiates through the hohlraum to compress the capsule of fusion fuel. Iron radiation shims are used to enhance symmetry of the fuel's compression.

One novel design features a gold cone attached to the spherical shell enclosing the deuterium–tritium fuel. The cone penetrates almost to the center of the capsule. In this way, the petawatt pulse has direct access to the ignition region. “The cone provides a clear path for the petawatt laser so that its energy can be deposited within about 100 micrometers or less of the high-density core,” explains Tabak. The design team is exploring variations in cone designs to reduce the distance between the capsule’s ignition region and the apex of the cone.

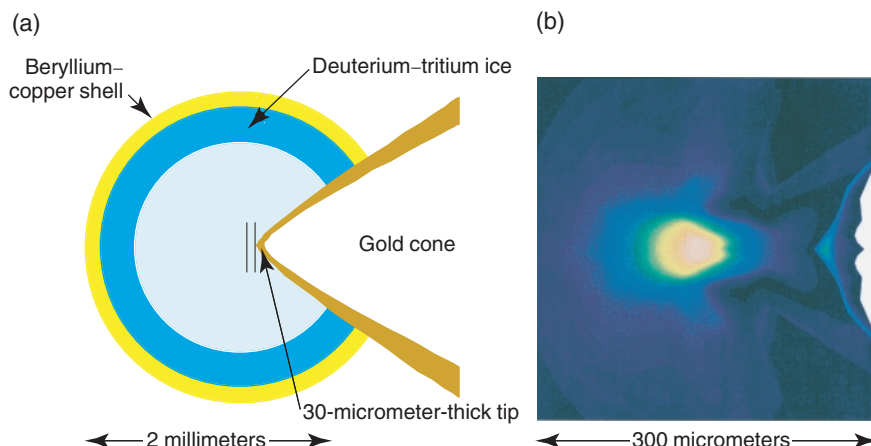
Fast-ignition simulations, combined with recent experiments in Japan and on the Omega laser at the University of Rochester, continue to show considerable promise for the concept. The experiments on Omega use prototype capsules designed by Lawrence Livermore physicist Steve Hatchett and manufactured by General Atomics. One series of experiments is showing scientists how the presence of a cone on the target affects the compression of fusion fuel.

Livermore target designs continue to evolve as the design team gains insight from experiments, simulations, and advances in the theoretical underpinnings of fast ignition and heavy-ion beams. The team is motivated by the steady progress its work is making toward eventual deployment of a fusion power plant. Whatever inertial fusion method is ultimately selected for commercial development, it will be using minuscule targets that are precisely designed.

—Arnie Heller

**Key Words:** fast ignition, heavy-ion fusion, hohlraum, inertial fusion energy, laser fusion, Omega laser, petawatt laser.

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(a) In this design for a fast-ignition target, a gold cone is attached to the beryllium–copper spherical shell enclosing deuterium–tritium fusion fuel. The cone penetrates almost to the center of the capsule to allow a petawatt laser to directly deposit its energy to the compressed fuel. (b) A computer simulation of the target fuel being ignited by a petawatt laser. The fuel has a hollow core and is located about 100 micrometers from the tip of the cone.

## Patents

### Manifold Free Multiple Sheet Superplastic Forming

**John W. Elmer, Robert L. Bridges**

U.S. Patent 6,264,880 B1

July 24, 2001

Fluid-forming compositions in a container attached to enclosed adjacent sheets are heated to relatively high temperatures to generate fluids (gases) that effect inflation of the sheets. Fluid rates to the enclosed space between the sheets can be regulated by the canal from the container. Inflated articles can be produced by a continuous, rather than a batch, process.

### Kit for Detecting Nucleic Acid Sequences Using Competitive Hybridization Probes

**Joe N. Lucas, Tore Straume, Kenneth T. Bogen**

U.S. Patent 6,270,972 B1

August 7, 2001

A kit for detecting a target nucleic acid sequence in a sample. The kit contains four hybridization probes. A first hybridization probe includes a nucleic acid sequence that is sufficiently complementary to selectively hybridize to a first portion of the target sequence. The first hybridization probe includes a first complexing agent for forming a binding pair with a second complexing agent. A second hybridization probe includes a nucleic acid sequence that is complementary to selectively hybridize to a second portion of the target sequence to which the first hybridization probe does not selectively hybridize. The second hybridization probe includes a detectable marker. A third hybridization probe includes a nucleic acid sequence that is sufficiently complementary to selectively hybridize to a first portion of the target sequence. The third probe includes the same detectable marker as the second hybridization probe. A fourth hybridization probe includes a nucleic acid sequence that is sufficiently complementary to selectively hybridize to a second portion of the target sequence to which the third hybridization probe does not selectively hybridize. The fourth probe includes the first complexing agent for forming a binding pair with the second complexing agent.

The first and second hybridization probes are capable of simultaneously hybridizing to the target sequence, and the third and fourth hybridization probes are capable of simultaneously hybridizing to the target sequence. The detectable marker is not present on the first or fourth hybridization probes, and the first, second, third, and fourth hybridization probes include a competitive nucleic acid sequence sufficiently complementary to a

third portion of the target sequence that the competitive sequences of the first, second, third, and fourth hybridization probes compete with each other to hybridize to the third portion of the target sequence.

### Microfluidic Interconnects

**William J. Benett, Peter A. Krulevitch**

U.S. Patent 6,273,478 B1

August 14, 2001

A miniature connector for introducing microliter quantities of solutions into microfabricated fluidic devices. It incorporates a molded ring or seal set into a ferrule cartridge, with or without a compression screw. The fluidic connector, for example, joins standard high-pressure liquid chromatography tubing to 1-millimeter-diameter holes in silicon or glass, enabling milliliter-size volumes of sample solutions to be merged with microliter devices. The connector has many features, including ease of connecting and disconnecting; a small footprint that enables numerous connectors to be located in a small area; low dead volume; helium leak-tightness; and tubing that does not twist during connection. The connector thus enables easy and effective change of microfluidic devices and introduction of different solutions in the devices.

### High Efficiency Replicated X-Ray Optics and Fabrication Method

**Troy W. Barbee, Jr., Stephen M. Lane, Donald E. Hoffman**

U.S. Patent 6,278,764 B1

August 21, 2001

Replicated x-ray optics are fabricated by sputter deposition of reflecting layers on a super-polished reusable mandrel. The reflecting layers are strengthened by a supporting multilayer that results in stronger stress-relieved reflecting surfaces that do not deform during separation from the mandrel. The supporting multilayer enhances the ability to part the replica from the mandrel without degradation in surface roughness. The reflecting surfaces are comparable in smoothness to the mandrel surface. An outer layer is electrodeposited on the supporting multilayer. A parting layer may be deposited directly on the mandrel before the reflecting surface to facilitate removal of the layered, tubular optics device from the mandrel without deformation. The inner reflecting surface of the shell can be a single-layer grazing-reflection mirror or a resonant multilayer mirror. The resulting optics can be used in a variety of applications, including lithography, microscopy, radiography, tomography, and crystallography.

**Highly Charged Ion Based Time of Flight Emission Microscope****Alan V. Barnes, Thomas Schenkel, Alex V. Hamza, Dieter H. Schneider, Barney Doyle**

U.S. Patent 6,288,394 B1

September 11, 2001

A highly charged ion-based time-of-flight emission microscope that improves the surface sensitivity of static secondary-ion mass-spectrometer measurements because of the higher ionization probability of highly charged ions. Slow, highly charged ions are produced in an electron-beam ion trap and directed to the sample surface. The sputtered secondary ions and electrons pass through a specially designed objective lens to a microchannel plate detector. This new instrument permits high surface sensitivity (10 billion atoms per square centimeter), high spatial resolution (100 nanometers), and chemical structural information because of the high molecular ion yields. The high secondary ion yield permits coincidence counting, which can be used to enhance determination of chemical and topological structure and to correlate specific molecular species.

**High Sensitivity Charge Amplifier for Ion Beam Uniformity Monitor****Gary W. Johnson**

U.S. Patent 6,288,402 B1

September 11, 2001

An ion-beam-uniformity monitor for low beam currents using a high-sensitivity charge amplifier with bias compensation. The ion-beam monitor is used to assess the uniformity of a raster-scanned ion beam, such as that in an ion implanter. The monitor includes four Faraday cups placed in the geometric corners of the target area. Current from each cup is integrated with respect to time, thus measuring accumulated dose, or charge, in coulombs. By comparing the dose at each corner, researchers can make a qualitative assessment of ion-beam uniformity. With knowledge of the relative area of the Faraday cups, the ion flux and areal dose can also be obtained.

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**Awards**

At the American Vacuum Society's 48th International Symposium held in San Francisco, California, in late October, **Eli Rotenberg**, a staff scientist at the Laboratory, received the **Peter Mark Memorial Award** for "furthering our knowledge of nanophase and reduced dimensionality systems by creative use of angle-resolved photoemission." The symposium was held in conjunction with the International Union for Vacuum Science, Technique, and Application's 15th International Vacuum Congress and the 11th International Conference on Solid Surfaces.

Nuclear engineer **Craig Smith** has become a **fellow** of the **American Nuclear Society**. Smith was honored for his outstanding accomplishments in the field of nuclear

health, safety, and regulation as well as for his work in radiation protection and waste management. He has 30 years of experience in the nuclear and environmental fields and is leader of the Laboratory's Fission Energy and Systems Safety program. In this position, Smith oversees research in nuclear technology and system safety; the Argus security system for nuclear facilities, Livermore, and other laboratories; and the Laboratory's support to the Department of Energy in monitoring the purchase of highly enriched uranium from Russia. Smith has also led several collaborative projects with research institutes in the former Soviet Union.



## Abstracts

### Welding Science: A New Look at a Fundamental Technology

Livermore has a vital interest in knowing all it can about welding. Dependable welds are important for maintaining the performance and safety of nuclear weapons. Welds will also play a key role in the success of the Department of Energy's planned repository for long-term storage of nuclear wastes, which is being investigated through the Yucca Mountain project. In experiments using synchrotron radiation and x-ray diffraction, a Livermore team has succeeded in producing the first-ever maps of real-time microstructural changes that occur in and around the weld area as a metal melts and resolidifies. More recently, their experiments have revealed second-by-second changes in a metal's microstructure during welding. Results of recent time-resolved experiments indicated that nonequilibrium solidification of welds can occur, affecting weld reliability. These data are now being used by others to design new self-shielded welding electrodes with improved weld properties.

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**Joe Wong** (925) 423-6385 ([wong10@llnl.gov](mailto:wong10@llnl.gov)).

### Probing the Subsurface with Electromagnetic Fields

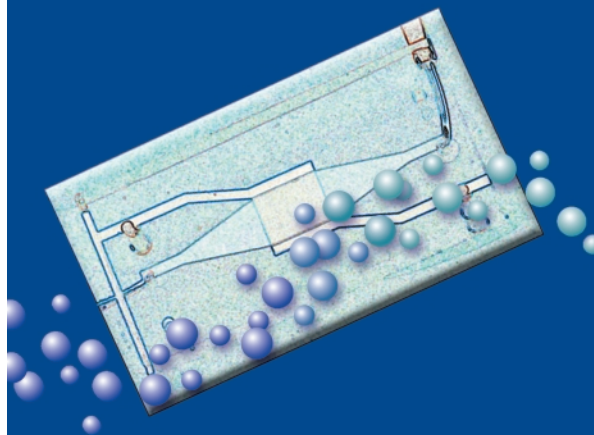
Lawrence Livermore researchers have been working with U.S. oil companies to improve enhanced oil recovery technologies so that more oil can be extracted from domestic production fields. One promising method is to inject carbon dioxide underground to force more oil to the surface. A technique to view underground fluids and gases, called crosswell electromagnetic imaging, is a valuable tool for monitoring enhanced oil recovery operations. The technology provides high-resolution images of underground deposits of oil, water, gas, and other materials by measuring electrical resistivity or conductivity of electrical current passing through different materials. The technique is being tested by Lawrence Livermore researchers at a central California oil field. The technology could be extended to monitoring underground sequestration (long-term storage) of carbon dioxide from industrial operations, a technique that is being explored to help the environment.

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## Simulation-Aided Design of Microfluidic Devices



A comprehensive model of particle interactions in the channels of microfluidic devices will improve and speed up the design of these devices, which are important to medical, chemical, and pharmaceutical research.

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